Photoredox-Catalyzed Synthesis of Sulfonated Oxazolines from *N*-allylamides through the Insertion of Sulfur Dioxide

Zhichao Chen,[a] Hong Zhang,[b] Shu-Feng Zhou,*[,a] and Xiuling Cui*[,b]

[a]*College of Chemical Engineering, Huaqiao University, Xiamen, Fujian 361021, P. R. China.*
[b]*Engineering Research Centre of Molecular Medicine of Ministry of Education, Key Laboratory of Fujian Molecular Medicine, Key Laboratory of Precision Medicine and Molecular Diagnosis of Fujian Universities, Key Laboratory of Xiamen Marine and Gene Drugs, School of Biomedical Sciences, Huaqiao University, Xiamen 361021, P. R. China.*

Corresponding Author: Xiuling Cui and Shu-Feng Zhou

Email: cuixl@hqu.edu.cn

Email: szhou@hqu.edu.cn

Tel & Fax: +86-592-6162996

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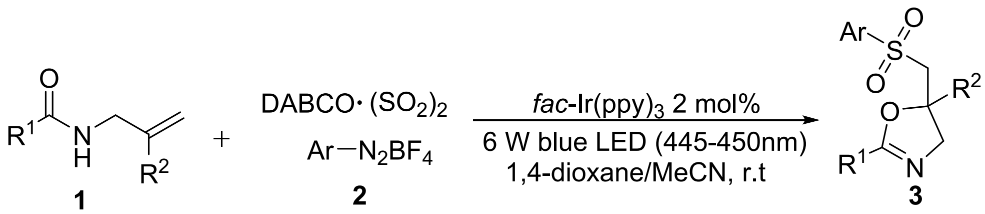
1. General information

Unless otherwise stated, all commercial materials and solvents were used directly without further purification. ^{1}H and ^{13}C NMR spectra were measured on a 400 MHz Bruker spectrometer (^{1}H 400MHz, ^{13}C 100MHz, ^{19}F NMR 376 MHz), using $CDCl_3$ (spectra were referenced to the solvent peaks ^{1}H: residual $CDCl_3$ = 7.26 ppm, ^{13}C: $CDCl_3$ = 77.0 ppm) or DMSO-d_6 (spectra were referenced to the solvent peaks ^{1}H: residual DMSO-d_6 = 2.50 ppm, ^{13}C: DMSO-d_6 = 39.5 ppm) as the solvent. High-resolution mass spectra (HRMS) were measured on ESI-TOF. Column chromatography was performed on silica gel (70-230 mesh ASTM) using the reported eluent. Thin-layer chromatography (TLC) was carried out on 4×5 cm plates with a layer thickness of 0.2 mm (silica gel 60 F254). Photochemical reactions were performed with a LED reactor WP-TEC-1020HSL (WATTCAS, China). Starting materials aryldiazonium tetrafluoroborates **2,** *N*-allylamides **1** were prepared according to the literatures.[S1, S2]

2. General catalytic procedure for the synthesis of 3

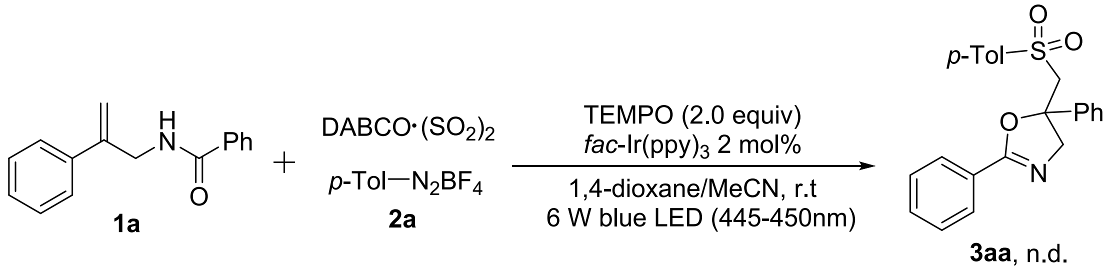


N-Allylamides **1** (0.2 mmol), aryldiazonium tetrafluoroborates **2** (0.4 mmol), DABCO•$(SO_2)_2$ (0.2 mmol, 1 equiv), *fac*-$Ir(ppy)_3$ (2 mol%), and 2 mL 1,4-dioxane/MeCN (3:1) were added in a quartz tube. Then the mixture was stirred at rt for 12 h in the photochemical reactor with 6 W blue LED as light source under N_2 atmosphere. After completion of the *N*-allylamides, the solvent was removed under reduced pressure by rotary evaporator. Then, the residue was purified by silica gel column chromatography to give the desired products **3**.

Figure. S1 The WP-TEC-1020HSL photochemical reaction system with the blue light LED

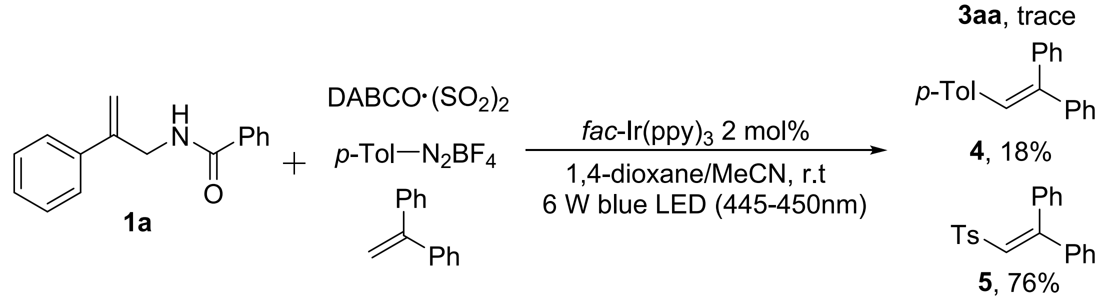
3. Mechanism Exploration

(1) Trapping experiment with 2,2,6,6-tetramethylpiperidin-1-oxyl (TEMPO)



N-Allylamide **1a** (0.2 mmol), 4-methylphenyldiazonium tetrafluoroborate **2a** (0.4 mmol), DABCO•$(SO_2)_2$ (0.2 mmol, 1 equiv), *fac*-Ir(ppy)$_3$ (2 mol%), TEMPO (0.4 mmol, 2.0 equiv) and 2 mL 1,4-dioxane/MeCN (3:1) were added in a quartz tube. Then the mixture was stirred at rt for 12 h in the photochemical reactor with 6 W blue LED as light source under N_2 atmosphere. The resulting mixture was monitored by TLC.

(2) Trapping experiment with ethene-1,1-diyldibenzene



N-Allylamide **1a** (0.2 mmol), 4-methylphenyldiazonium tetrafluoroborate **2a** (0.4 mmol), DABCO•$(SO_2)_2$ (0.2 mmol, 1 equiv), *fa*c-Ir(ppy)$_3$ (2 mol%), ethene-1,1-diyldibenzene (0.2 mmol, 1.0 equiv) and 2 mL 1,4-dioxane/MeCN (3:1) were added in a quartz tube. Then the mixture was stirred at rt for 12 h in the photochemical reactor with 6 W blue LED as light source under N_2 atmosphere. The solvent was removed under reduced pressure, purification was performed by flash column chromatography on silica gel with petroleum ether/ethyl acetate as eluent to give the corresponding compounds **4** and **5**.

(3) Stern-volmer studies

A Hitachi F-7000 fluoresence spectrometer was used to record the emission intensities. All the solutions were excited at 463 nm and the emission intensity at 518 nm was observed. 1,4-dioxane/MeCN (3:1) was degassed with a stream of Ar for 15 min. In a typical experiment, the emission spectrum of a 1.0×10^{-3} M solution of *fac*-Ir(ppy)$_3$ in 1,4-dioxane/MeCN (3:1) was collected. Then, appropriate amount of quencher **1a** was added to the measured solution in a quartz cuvette and the emission spectrum of the sample was collected. I_0 and I represent the intensities of the emission in the absence and presence of the quencher at 518 nm. The results were presented in Figure S2 and Figure S3.

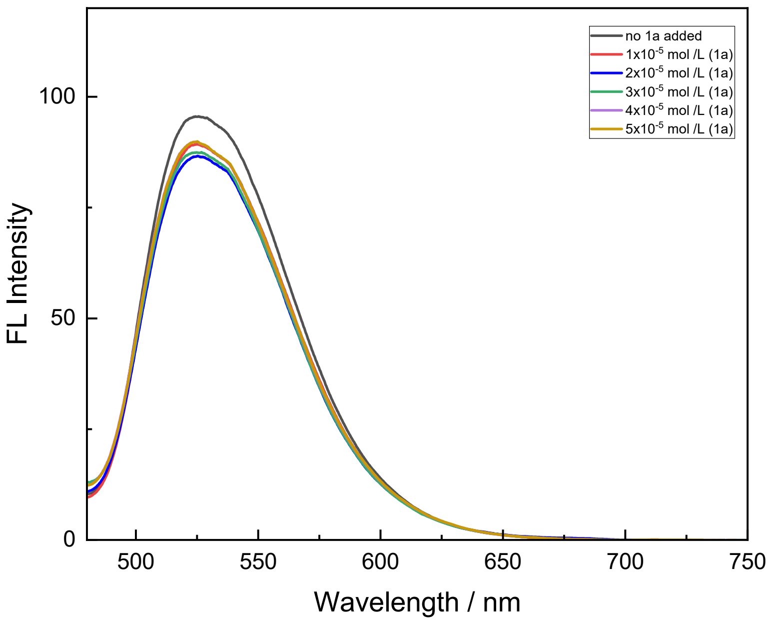


Figure S2 Quenching of *fac*-Ir(ppy)$_3$ fluorescence emission in the presence of *N*-allylbenamide **1a**.

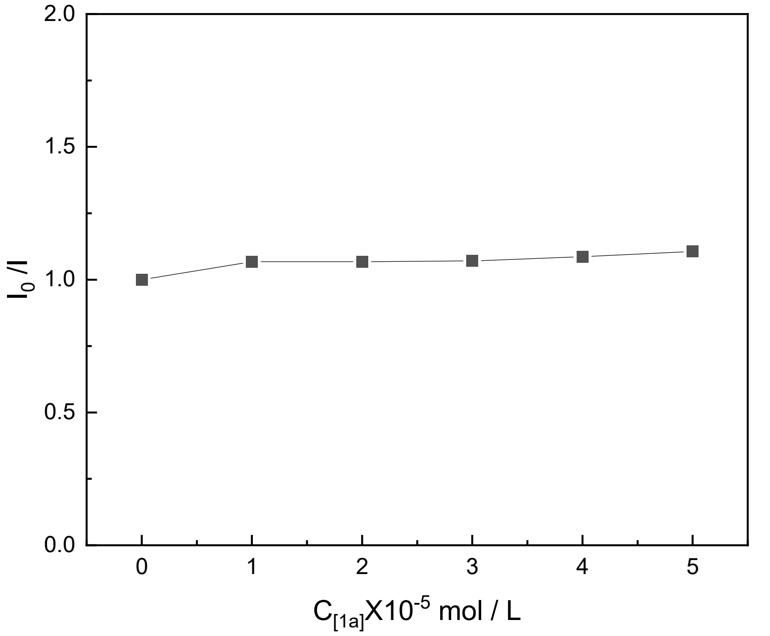


Figure S3 Stern-volmer plots.

A Hitachi F-7000 fluoresence spectrometer was used to record the emission intensities. All the solutions were excited at 463 nm and the emission intensity at 518 nm was observed. 1,4-dioxane/MeCN (3:1) was degassed with a stream of Ar for 15 min. In a typical experiment, the emission spectrum of a 1.0×10^{-3} M solution of *fac*-Ir(ppy)$_3$ in 1,4-dioxane/MeCN (3:1) was collected. Then, appropriate amount of quencher **2a** was added to the measured solution in a quartz cuvette and the emission spectrum of the sample was collected. I_0 and I represent the intensities of the emission in the absence and presence of the quencher at 518 nm. The results were presented in Figure S4 and Figure S5.

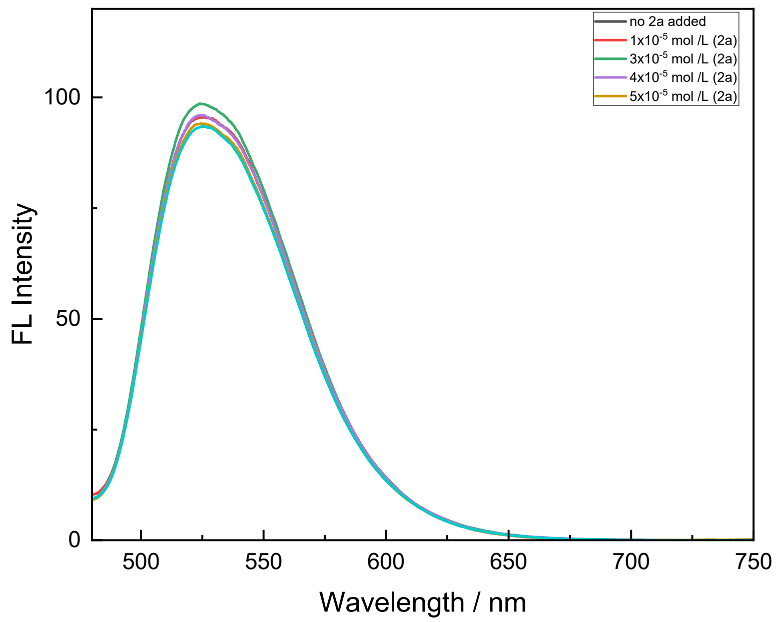


Figure S4 Quenching of *fac*-Ir(ppy)$_3$ fluorescence emission in the presence of aryldiazonium tetrafluoroborate **2a**.

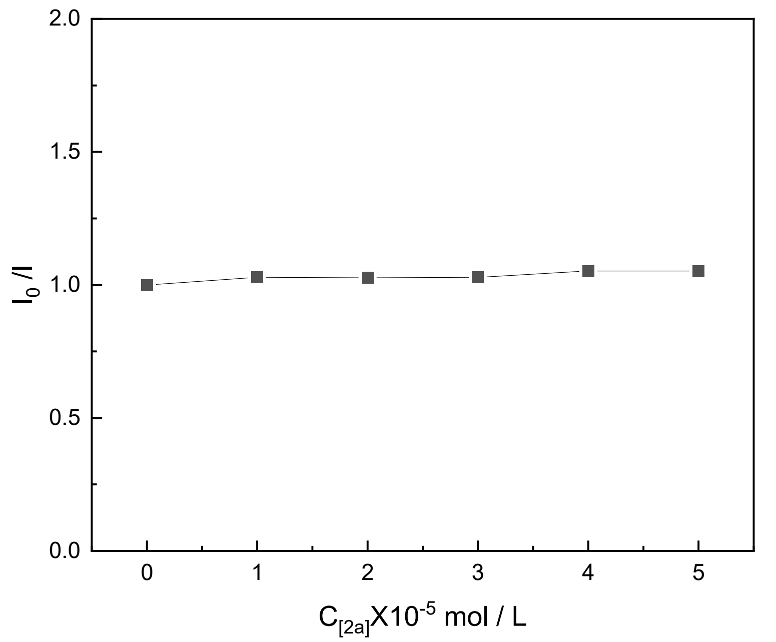


Figure S5 Stern-volmer plots.

A Hitachi F-7000 fluoresence spectrometer was used to record the emission intensities. All the solutions were excited at 463 nm and the emission intensity at 518 nm was observed. 1,4-dioxane/MeCN (3:1) was degassed with a stream of Ar for 15 min. In a typical experiment, the emission spectrum of a 1.0×10^{-3} M solution of *fac*-Ir(ppy)$_3$ in 1,4-dioxane/MeCN (3:1) was collected. Then, appropriate amount of quencher **DABCO•(SO$_2$)$_2$** was added to the measured solution in a quartz cuvette and the emission spectrum of the sample was collected. I_0 and I represent the intensities of the emission in the absence and presence of the quencher at 518 nm. The results were presented in Figure S6 and Figure S7.

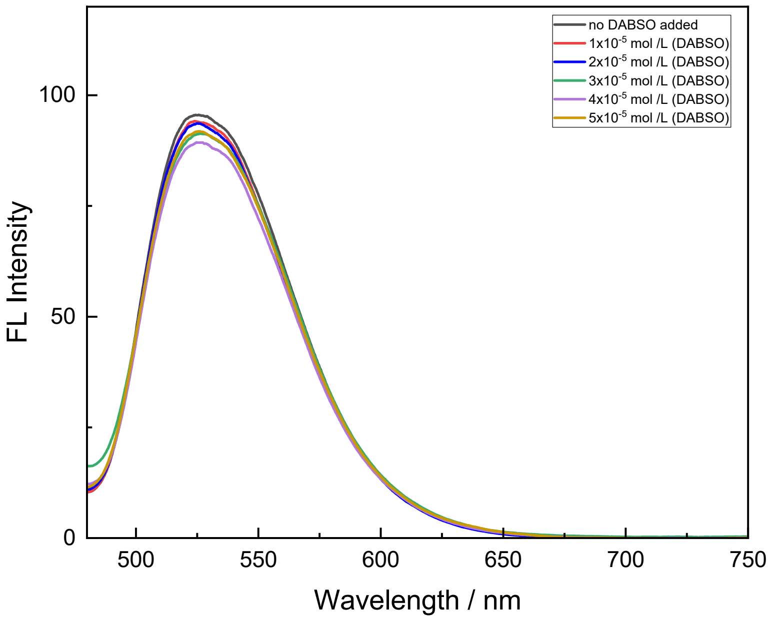


Figure S6 Quenching of *fac*-Ir(ppy)$_3$ fluorescence emission in the presence of **DABCO•(SO$_2$)$_2$**.

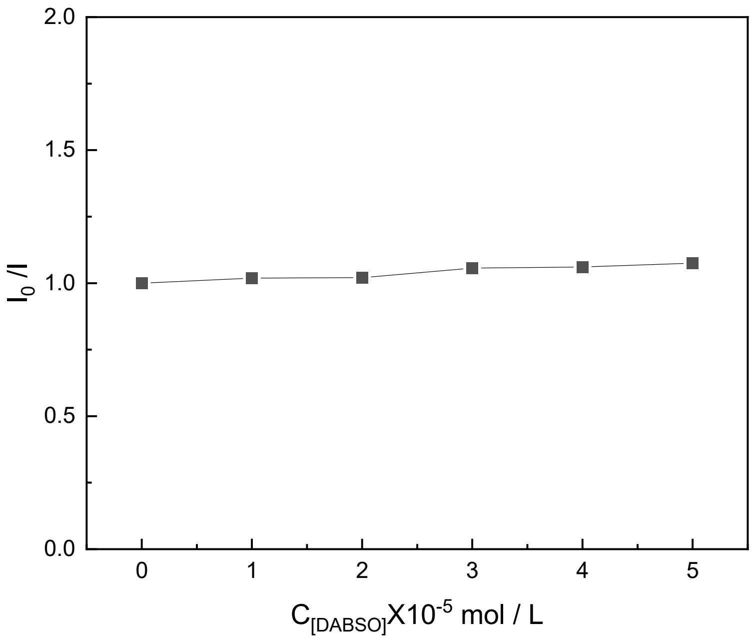


Figure S7 Stern-volmer plots.

A Hitachi F-7000 fluoresence spectrometer was used to record the emission intensities. All the solutions were excited at 463 nm and the emission intensity at 518 nm was observed. 1,4-dioxane/MeCN (3:1) was degassed with a stream of Ar for 15 min. In a typical experiment, the emission spectrum of a 1.0×10^{-3} M solution of *fac*-Ir(ppy)$_3$ in 1,4-dioxane/MeCN (3:1) was collected. Then, appropriate amount of quencher (mixture of **DABCO•(SO$_2$)$_2$** and *N*-allylbenamide **1a)** was added to the measured solution in a quartz cuvette and the emission spectrum of the sample was collected. I_0 and I represent the intensities of the emission in the absence and presence of the quencher at 518 nm. The results were presented in Figure S8 and Figure S9.

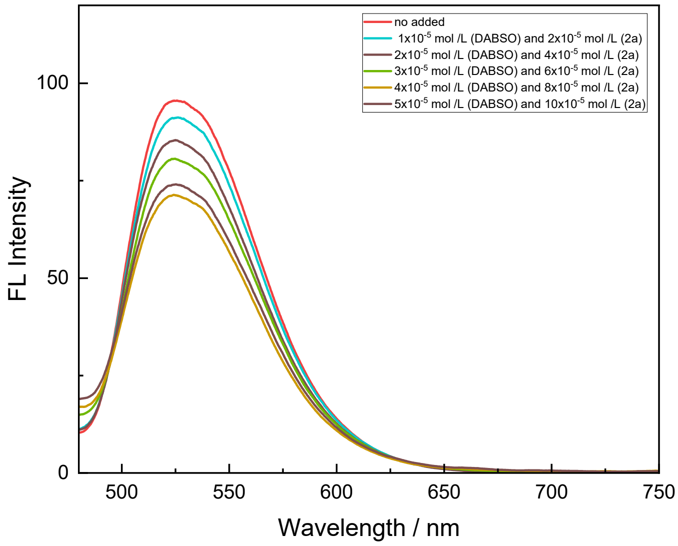


Figure S8 Quenching of *fac*-Ir(ppy)$_3$ fluorescence emission in the presence of aryldiazonium tetrafluoroborate **2a** and DABCO•(SO$_2$)$_2$.

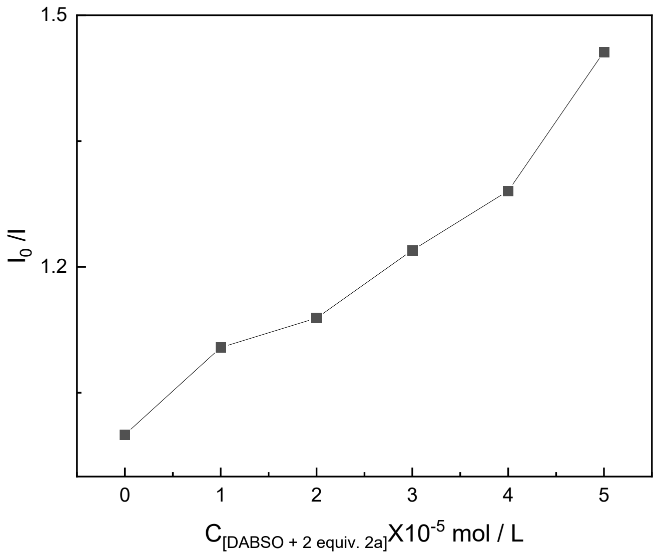
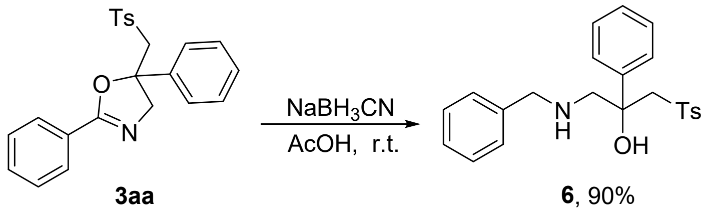


Figure S9 Stern-volmer plots.

4. Derivatization of 3aa



To a stirred solution of **3aa** (0.2 mmol, 1.0 equiv.) in 2.0 mL of AcOH, was added 64 mg of $NaBH_3CN$ (1.0 mmol, 5 equiv.). After stirring the reaction overnight, 2.0 mL of H_2O was added dropwise. After an additional hour, the reaction was diluted with DCM (40 mL), and neutralized with saturated $NaHCO_3$. The aqueous layer was extracted three times with DCM (40 mL each). The combined organic phase was dried with Na_2SO_4, filtered, and solvent vas removed in vacuo. The product was purified by column chromatography on silica gel to yield 71.2 mg (90%) of pure **6** as a white solid.

5. Large-scale synthesis of oxazoline 3aa

N-Allylamide **1a** (2 mmol), 4-methylphenyldiazonium tetrafluoroborate **2a** (4 mmol), DABCO•$(SO_2)_2$ (2 mmol, 1 equiv), *fac*-Ir$(ppy)_3$ (2 mol%), and 5 mL 1,4-dioxane/MeCN (3:1) were added in a quartz tube. Then the mixture was stirred at rt for 24 h in the photochemical reactor with 6 W blue LED as light source under N_2 atmosphere. After completion of the *N*-allylamides, the solvent was removed under reduced pressure by rotary evaporator. Then, the residue was purified by silica gel column chromatography to give the desired product **3aa**.

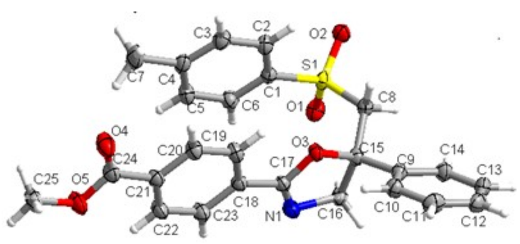
6. References

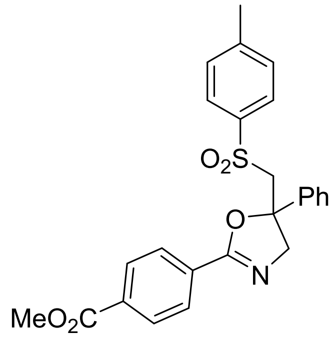
[S1] (a) Wang, Pan.; Yang, Z.; Wang, Z.; Xu, C.; Huang, L.; Wang, S.; Zhang, H.; Lei, A. *Angew. Chem., Int. Ed.* **2019**, *58*, 15747-15751. (b) Zhang, N.; Quan, Z.-J.; Zhang, Z.; Da, Y.-X.; Wang, X.-C. *Chem. Commun.* **2016**, *52*, 14234-14237.

[S2] (a) Zhang, X. W.; Cao, B. N.; Yu, S. C.; Zhang, X. M. *Angew. Chem. Int. Ed.* **2010**, *49*, 4047-4050. (b) Yu, J.; Yang, H.; Fu, H. *Adv. Synth. Catal.* **2014**, *356*, 3669-3675.

7. X-ray data of compound 3ga:

Single crystal suitable for X-ray diffraction experiment was obtained by slow evaporation of DCM/*n*-hexane (1:10, V/V) solution containing the compound **3ga.**





3ga **3ga**

Figure S1. X-ray molecular structure of 3ga with the probability at 50% level.

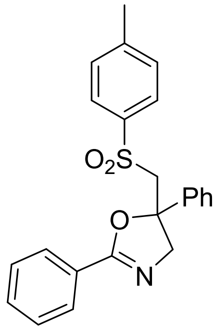
Table 1 Crystal data and structure refinement for 3ga.

Empirical formula	$C_{26}H_{18}F_3NO_3S$
Formula weight	481.47
Temperature/K	293(2)
Crystal system	monoclinic
Space group	C2/c
a/Å	42.2841(7)
b/Å	6.85075(14)
c/Å	15.5747(3)
α/°	90
β/°	92.6612(16)
γ/°	90
Volume/Å3	4506.77(15)
Z	8
ρcalcg/cm3	1.419
μ/mm 1	1.757
F(000)	1984.0
Crystal size/mm3	0.15 × 0.12 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.374 to 134.134
Index ranges	$-42 \leq h \leq 50$, $-8 \leq k \leq 8$, $-18 \leq l \leq 18$
Reflections collected	15430
Independent reflections	4027 [R_{int} = 0.0275, R_{sigma} = 0.0211]
Data/restraints/parameters	4027/21/318
Goodness-of-fit on F2	1.060
Final R indexes [I>=2σ (I)]	R_1 = 0.0485, wR_2 = 0.1320
Final R indexes [all data]	R_1 = 0.0528, wR_2 = 0.1366
Largest diff. peak/hole / e Å-	0.40/-0.37

3

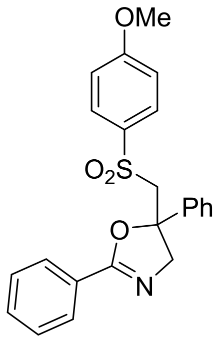
8. Characterization of compounds 3, 4, 5 and 6.

2,5-Diphenyl-5-(tosylmethyl)-4,5-dihydrooxazole (3aa)



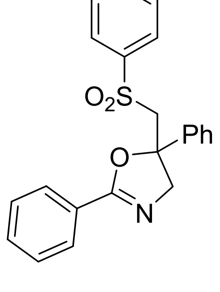
White solid. 64.1 mg, Yield: 82%, mp 108-109 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 7.5 Hz, 2H), 7.64 (d, J = 7.6 Hz, 2H), 7.50 (t, J = 7.3 Hz, 1H), 7.39 (t, J = 7.5 Hz, 2H), 7.36 – 7.25 (m, 5H), 7.13 (d, J = 7.7 Hz, 2H), 4.86 (d, J = 15.1 Hz, 1H), 4.21 (d, J = 15.1 Hz, 1H), 3.99 (d, J = 15.1 Hz, 1H), 3.88 (d, J = 15.1 Hz, 1H), 2.31 (s, 3H). ^{13}C NMR (100MHz, $CDCl_3$) δ 162.3, 144.5, 142.4, 137.3, 131.6, 129.7, 128.8, 128.3, 128.2, 128.2, 128.1, 127.0, 124.4, 85.1, 66.7, 64.3, 21.5. HRMS (ESI) *m/z* calcd for $C_{23}H_{21}NO_3S$ $[M+H]^+$ 392.1315, found 392.1317.

5-(((4-Methoxyphenyl)sulfonyl)methyl)-2,5-diphenyl-4,5-dihydrooxazole (3ab)



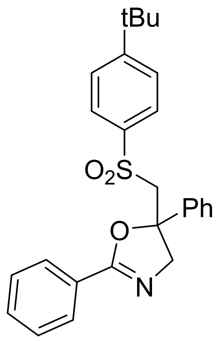
White solid. 67.6 mg, Yield: 83%, mp 118-119 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, J = 7.2 Hz, 2H), 7.67 (d, J = 8.9 Hz, 2H), 7.49 (d, J = 7.4 Hz, 1H), 7.39 (t, J = 7.7 Hz, 2H), 7.36 – 7.28 (m, 5H), 6.77 (d, J = 8.9 Hz, 2H), 4.86 (d, J = 15.1 Hz, 1H), 4.21 (d, J = 15.1 Hz, 1H), 3.98 (d, J = 15.1 Hz, 1H), 3.87 (d, J = 15.1 Hz, 1H), 3.74 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.6, 162.2, 142.5, 131.7, 131.6, 130.2, 128.8, 128.2, 128.2, 128.1, 127.1, 124.4, 114.2, 85.1, 66.6, 64.4, 55.5. HRMS (ESI) *m/z* calcd for $C_{23}H_{21}NO_4S$ $[M+H]^+$ 408.1264, found 408.1265.

2,5-Diphenyl-5-((phenylsulfonyl)methyl)-4,5-dihydrooxazole (3ac)



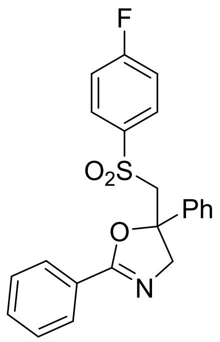
White solid. 55.8 mg, Yield: 74%, mp 113-114 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (dd, J = 13.8, 7.9 Hz, 4H), 7.50 (dd, *J* = 14.2, 7.1 Hz, 2H), 7.44 – 7.25 (m, 9H), 4.82 (d, *J* = 15.1 Hz, 1H), 4.24 (d, *J* = 15.1 Hz, 1H), 4.02 (d, *J* = 15.1 Hz, 1H), 3.92 (d, *J* = 15.1 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.3, 142.1, 140.4, 133.4, 131.7, 129.0, 128.8, 128.3, 128.3, 128.2, 128.0, 127.0, 124.5, 85.0, 67.0, 64.2. HRMS (ESI) *m/z* calcd for $C_{22}H_{19}NO_3S$ $[M+Na]^+$ 400.0978, found 400.0979.

5-(((4-(Tert-butyl)phenyl)sulfonyl)methyl)-2,5-diphenyl-4,5-dihydrooxazole (3ad)



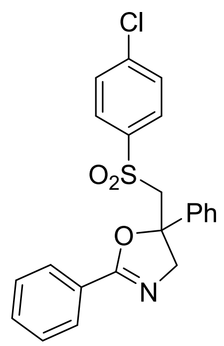
White solid. 58.9 mg, Yield: 68%, mp 163-164 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.8 Hz, 2H), 7.66 (d, *J* = 8.0 Hz, 2H), 7.51 (t, *J* = 7.3 Hz, 1H), 7.39 (dd, *J* = 18.5, 7.9 Hz, 4H), 7.34 – 7.26 (m, 5H), 4.85 (d, *J* = 15.1 Hz, 1H), 4.24 (d, *J* = 15.1 Hz, 1H), 4.01 (d, *J* = 15.1 Hz, 1H), 3.90 (d, *J* = 15.1 Hz, 1H), 1.28 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4, 157.3, 142.2, 137.2, 131.6, 128.7, 128.4, 128.3, 128.1, 127.9, 127.1, 126.0, 124.5, 85.1, 66.9, 64.2, 35.1, 31.0. HRMS (ESI) *m/z* calcd for $C_{26}H_{27}NO_3S$ $[M+H]^+$ 434.1784, found 434.1785.

5-(((4-Fluorophenyl)sulfonyl)methyl)-2,5-diphenyl-4,5-dihydrooxazole (3ae)



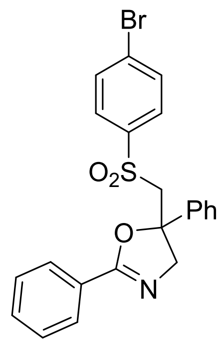
White solid. 60.8 mg, Yield: 77%, mp 127-128 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.3 Hz, 2H), 7.77 – 7.70 (m, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.37 – 7.27 (m, 5H), 7.00 (t, *J* = 8.6 Hz, 2H), 4.80 (d, *J* = 15.1 Hz, 1H), 4.22 (d, *J* = 15.1 Hz, 1H), 4.01 (d, *J* = 15.2 Hz, 1H), 3.91 (d, *J* = 15.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6 (d, *J* = 256.3 Hz), 162.2, 142.0, 136.3 (d, *J* = 3.1 Hz), 131.8, 131.0 (d, *J* = 9.7 Hz), 128.9, 128.4, 128.3, 128.2, 126.9, 124.4, 116.3 (d, *J* = 22.7 Hz), 85.0, 67.1, 64.4. ^{19}F NMR (376 MHz, $CDCl_3$) δ -103.74. HRMS (ESI) *m/z* calcd for $C_{22}H_{18}FNO_3S$ $[M+H]^+$ 396.1064, found 392.1067.

5-(((4-Chlorophenyl)sulfonyl)methyl)-2,5-diphenyl-4,5-dihydrooxazole (3af)



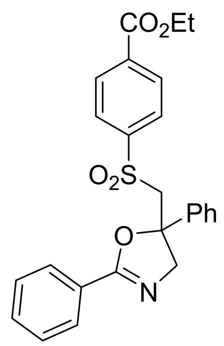
White solid. 64.1 mg, Yield: 78%, mp 134-136 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.3 Hz, 2H), 7.66 (d, *J* = 8.6 Hz, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.33 (ddd, *J* = 18.8, 8.4, 5.2 Hz, 7H), 4.80 (d, *J* = 15.1 Hz, 1H), 4.21 (d, *J* = 15.1 Hz, 1H), 4.02 (d, *J* = 15.2 Hz, 1H), 3.91 (d, *J* = 15.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2, 141.9, 140.2, 138.6, 131.8, 129.5, 129.3, 128.9, 128.4, 128.3, 128.1, 126.7, 124.4, 84.9, 67.1, 64.3. HRMS (ESI) *m/z* calcd for $C_{22}H_{18}ClNO_3S$ $[M+H]^+$ 412.0769, found 412.0770.

5-(((4-Bromophenyl)sulfonyl)methyl)-2,5-diphenyl-4,5-dihydrooxazole (3ag)



White solid. 61.9 mg, Yield: 68%, mp 130-131 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.8 Hz, 2H), 7.58 (d, *J* = 7.7 Hz, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.44 (dd, *J* = 16.4, 8.2 Hz, 4H), 7.37 – 7.27 (m, 5H), 4.79 (d, *J* = 15.1 Hz, 1H), 4.20 (d, *J* = 15.1 Hz, 1H), 4.02 (d, *J* = 15.3 Hz, 1H), 3.91 (d, *J* = 15.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2, 141.9, 139.1, 132.3, 131.9, 129.6, 128.9, 128.5, 128.3, 128.1, 126.7, 124.4, 84.9, 67.1, 64.2. HRMS (ESI) *m/z* calcd for $C_{22}H_{18}BrNO_3S$ $[M+H]^+$ 456.0264, found 456.0262.

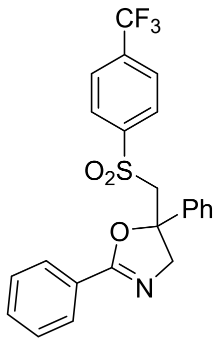
Ethyl 4-(((2,5-diphenyl-4,5-dihydrooxazol-5-yl)methyl)sulfonyl)benzoate (3ah)



White solid. 56.6 mg, Yield: 63%, mp 136-138 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.8 Hz, 2H), 7.80 (d, *J* = 7.9 Hz, 2H), 7.69 (d, *J* = 7.7 Hz, 2H), 7.47 (t, *J* = 7.3 Hz, 1H), 7.33 (dt, *J* = 11.8, 7.1 Hz,7H), 4.83 (d, *J* = 15.1 Hz, 1H), 4.40 (q, *J* = 7.0 Hz, 2H), 4.21 (d, *J* = 15.1 Hz, 1H), 4.05 (d, *J* = 15.3

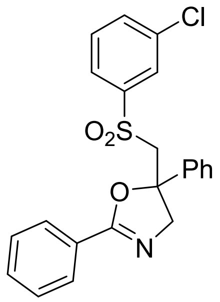
Hz, 1H), 3.94 (d, J = 15.3 Hz, 1H), 1.42 (t, J = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.9, 162.1, 143.7, 142.0, 134.8, 131.7, 130.1, 128.9, 128.3, 128.3, 128.2, 128.1, 126.7, 84.9, 66.9, 64.2, 61.7, 14.3. HRMS (ESI) *m/z* calcd for $C_{25}H_{23}NO_5S$ $[M+H]^+$ 450.1370, found 450.1371.

2,5-Diphenyl-5-(((4-(trifluoromethyl)phenyl)sulfonyl)methyl)-4,5-dihydrooxazole (3ai)



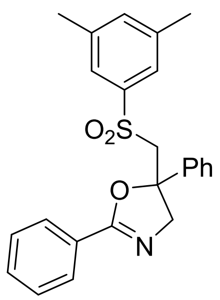
White solid. 53.4 mg, Yield: 60%, mp 143-144 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, J = 8.0 Hz, 2H), 7.70 (d, J = 7.8 Hz, 2H), 7.59 (d, J = 8.0 Hz, 2H), 7.51 (t, J = 7.4 Hz, 1H), 7.39 (t, J = 7.5 Hz, 2H), 7.30 (dd, J = 17.1, 7.3 Hz, 5H), 4.81 (d, J = 15.1 Hz, 1H), 4.22 (d, J = 15.1 Hz, 1H), 4.07 (d, J = 15.3 Hz, 1H), 3.97 (d, J = 15.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2, 143.5, 141.7, 135.0 (q, J = 32.9 Hz), 131.9, 128.9, 128.7, 128.4, 128.4, 128.0, 126.6, 126.1 (q, J = 3.4 Hz), 124.4, 123.0 (q, J = 273.8 Hz), 84.8, 67.1, 64.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.16 (s). HRMS (ESI) *m/z* calcd for $C_{23}H_{18}F_3NO_3S$ $[M+H]^+$ 446.1032, found 446.1034.

5-(((3-Chlorophenyl)sulfonyl)methyl)-2,5-diphenyl-4,5-dihydrooxazole (3aj)



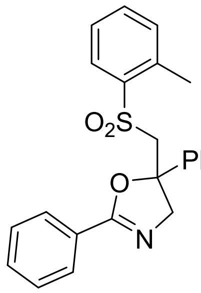
White solid. 50.2 mg, Yield: 61%, mp 103-104 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, J = 7.8 Hz, 2H), 7.68 (s, 1H), 7.62 (d, J = 7.8 Hz, 1H), 7.52 (t, J = 7.2 Hz, 1H), 7.42 (t, J = 7.6 Hz, 3H), 7.37 – 7.24 (m, 6H), 4.77 (d, J = 15.1 Hz, 1H), 4.23 (d, J = 15.1 Hz, 1H), 4.04 (d, J = 15.2 Hz, 1H), 3.94 (d, J = 15.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.3, 141.8, 141.6, 135.3, 133.6, 131.8, 130.3, 128.8, 128.4, 128.2, 126.7, 126.1, 124.5, 84.9, 67.2, 64.3. HRMS (ESI) *m/z* calcd for $C_{22}H_{18}ClNO_3S$ $[M+Na]^+$ 434.0588, found 434.0587.

5-(((3,5-Dimethylphenyl)sulfonyl)methyl)-2,5-diphenyl-4,5-dihydrooxazole (3ak)



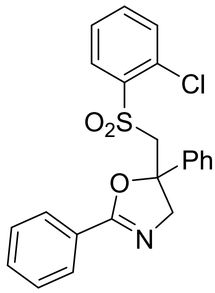
White solid. 64.8 mg, Yield: 80%, mp 132-133 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 7.8 Hz, 2H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.40 (t, *J* = 7.7 Hz, 2H), 7.36 – 7.27 (m, 7H), 7.06 (s, 1H), 4.89 (d, *J* = 15.1 Hz, 1H), 4.23 (d, *J* = 15.1 Hz, 1H), 4.01 (d, *J* = 15.1 Hz, 1H), 3.89 (d, *J* = 15.1 Hz, 1H), 2.22 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2, 142.4, 140.0, 139.1, 135.1, 131.6, 128.7, 128.2, 128.2, 128.2, 127.0, 125.5, 124.4, 85.0, 66.6, 64.2, 21.0. HRMS (ESI) *m/z* calcd for $C_{24}H_{23}NO_3S$ $[M+Na]^+$ 428.1291, found 428.1293.

2,5-Diphenyl-5-((*o*-tolylsulfonyl)methyl)-4,5-dihydrooxazole (3al)



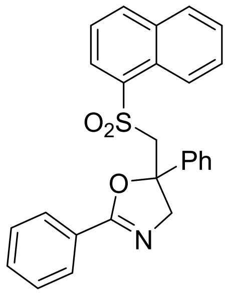
White solid. 55.5 mg, Yield: 71%, mp 109-110 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.9 Hz, 1H), 7.75 (d, *J* = 7.8 Hz, 2H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.42 – 7.28 (m, 8H), 7.17 (d, *J* = 7.5 Hz, 1H), 7.13 (t, *J* = 7.6 Hz, 1H), 4.86 (d, *J* = 15.1 Hz, 1H), 4.23 (d, *J* = 15.1 Hz, 1H), 4.05 (d, *J* = 15.1 Hz, 1H), 3.92 (d, *J* = 15.1 Hz, 1H), 2.65 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2, 142.3, 138.4, 137.6, 133.4, 132.5, 131.6, 130.1, 128.8, 128.2, 128.2, 126.8, 126.5, 124.4, 85.1, 66.8, 63.4, 20.4. HRMS (ESI) *m/z* calcd for $C_{23}H_{21}NO_3S$ $[M+H]^+$ 392.1315, found 392.1317.

5-(((2-Chlorophenyl)sulfonyl)methyl)-2,5-diphenyl-4,5-dihydrooxazole (3am)



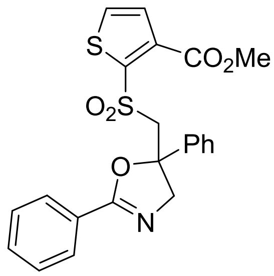
White solid. 57.6 mg, Yield: 70%, mp 112-114 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.9 Hz, 1H), 7.74 (d, *J* = 7.6 Hz, 2H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.41 – 7.22 (m, 9H), 7.14 (t, *J* = 7.6 Hz, 1H), 4.86 (d, *J* = 15.1 Hz, 1H), 4.43 (d, *J* = 15.3 Hz, 1H), 4.24 (d, *J* = 15.1 Hz, 1H), 4.12 (d, *J* = 15.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.1, 142.0, 137.5, 134.3, 131.6, 131.5, 131.5, 128.8, 128.3, 128.2, 128.2, 127.2, 126.7, 124.4, 84.9, 66.7, 62.2. HRMS (ESI) *m/z* calcd for $C_{22}H_{18}ClNO_3S$ $[M+Na]^+$ 434.0588, found 434.0590.

5-((Naphthalen-1-ylsulfonyl)methyl)-2,5-diphenyl-4,5-dihydrooxazole (3an)



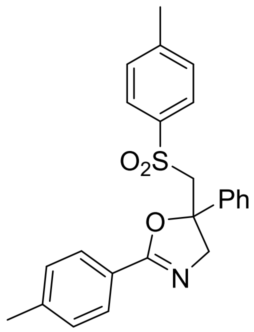
White solid. 60.7 mg, Yield: 71%, mp 120-121 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (d, *J* = 8.5 Hz, 1H), 8.06 (d, *J* = 7.2 Hz, 1H), 7.90 (t, *J* = 8.7 Hz, 2H), 7.70 – 7.56 (m, 4H), 7.48 (t, *J* = 7.1 Hz, 1H), 7.38 – 7.20 (m, 8H), 4.84 (d, *J* = 15.1 Hz, 1H), 4.36 – 3.98 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.3, 141.9, 135.0, 134.9, 134.1, 131.5, 130.8, 129.3, 128.8, 128.6, 128.2, 128.1, 126.8, 126.8, 124.4, 124.3, 123.8, 85.2, 66.9, 63.9. HRMS (ESI) *m/z* calcd for $C_{26}H_{21}NO_3S$ $[M+H]^+$ 428.1315, found 428.1314.

Methyl 2-(((2,5-diphenyl-4,5-dihydrooxazol-5-yl)methyl)sulfonyl)thiophene-3-carboxylate (3ao)



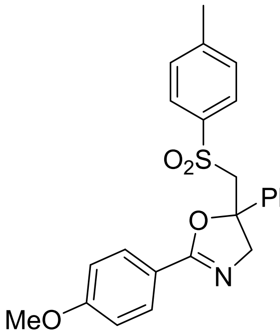
White solid. 29.1 mg, Yield: 33%, mp 132-133 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.9 Hz, 2H), 7.51 (t, *J* = 7.1 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.33 – 7.24 (m, 6H), 7.22 (d, *J* = 5.2 Hz, 1H), 4.81 (d, *J* = 15.0 Hz, 1H), 4.73 (d, *J* = 15.3 Hz, 1H), 4.35 (d, *J* = 15.2 Hz, 1H), 4.24 (d, *J* = 15.0 Hz, 1H), 3.90 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.3, 160.1, 144.4, 141.8, 133.6, 131.7, 131.5, 129.4, 128.6, 128.3, 128.2, 127.0, 124.5, 85.1, 67.3, 63.0, 53.1. HRMS (ESI) *m/z* calcd for $C_{22}H_{19}NO_5S_2$ $[M+Na]^+$ 464.0597, found 464.0598.

5-Phenyl-2-(p-tolyl)-5-(tosylmethyl)-4,5-dihydrooxazole (3ba)



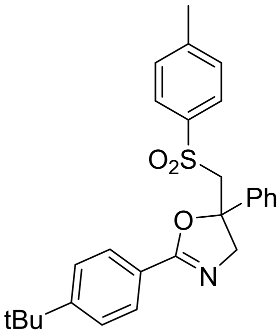
White solid. 56.7 mg, Yield: 70%, mp 127-129 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (dd, *J* = 7.4, 3.7 Hz, 4H), 7.38 – 7.26 (m, 5H), 7.19 (d, *J* = 7.8 Hz, 2H), 7.14 (d, *J* = 7.9 Hz, 2H), 4.83 (d, *J* = 15.0 Hz, 1H), 4.20 (d, *J* = 15.0 Hz, 1H), 3.99 (d, *J* = 15.1 Hz, 1H), 3.88 (d, *J* = 15.1 Hz, 1H), 2.42 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.5, 144.4, 142.4, 142.0, 137.3, 129.6, 128.9, 128.8, 128.3, 128.1, 128.1, 124.4, 124.2, 85.0, 66.6, 64.3, 21.6, 21.5. HRMS (ESI) *m/z* calcd for $C_{24}H_{23}NO_3S$ $[M+Na]^+$ 428.1291, found 428.1294.

2-(4-Methoxyphenyl)-5-phenyl-5-(tosylmethyl)-4,5-dihydrooxazole (3ca)



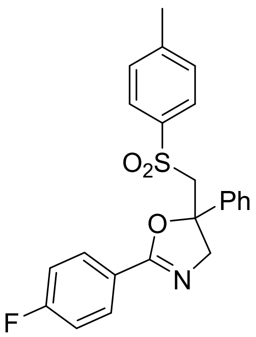
White solid. 57.3 mg, Yield: 60%, mp 168-170 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.3 Hz, 2H), 7.63 (d, *J* = 7.8 Hz, 2H), 7.38 – 7.27 (m, 5H), 7.15 (d, *J* = 7.9 Hz, 2H), 6.89 (d, *J* = 8.3 Hz, 2H), 4.80 (d, *J* = 14.9 Hz, 1H), 4.18 (d, *J* = 14.9 Hz, 1H), 3.98 (d, *J* = 15.1 Hz, 1H), 3.92 – 3.83 (m, 4H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.3, 162.1, 144.4, 142.4, 137.4, 130.0, 129.6, 128.7, 128.1, 124.4, 119.5, 113.6, 84.9, 66.7, 64.3, 55.4, 21.5. HRMS (ESI) *m/z* calcd for $C_{24}H_{23}NO_4S$ $[M+Na]^+$ 444.1240, found 444.1244.

2-(4-(Tert-butyl)phenyl)-5-phenyl-5-(tosylmethyl)-4,5-dihydrooxazole (3da)



White solid. 56.3 mg, Yield: 63%, mp 126-127 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (t, *J* = 9.7 Hz, 4H), 7.41 (d, *J* = 7.9 Hz, 2H), 7.36 – 7.24 (m, 5H), 7.13 (d, *J* = 7.7 Hz, 2H), 4.85 (d, *J* = 15.0 Hz, 1H), 4.19 (d, *J* = 15.1 Hz, 1H), 3.99 (d, *J* = 15.1 Hz, 1H), 3.87 (d, *J* = 15.1 Hz, 3H), 2.30 (s, 1H), 1.37 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.3, 155.1, 144.4, 142.6, 137.2, 129.7, 128.8, 128.1, 126.9, 125.6, 125.2, 124.4, 124.1, 84.9, 66.5, 64.2, 35.0, 31.2, 21.6. HRMS (ESI) *m/z* calcd for $C_{27}H_{29}NO_3S$ $[M+Na]^+$ 470.1760, found 470.1763.

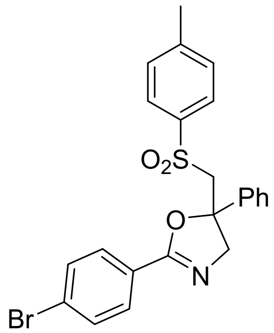
2-(4-Fluorophenyl)-5-phenyl-5-(tosylmethyl)-4,5-dihydrooxazole (3ea)



White solid. 59.7 mg, Yield: 73%, mp 149-150 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (dd, *J* = 7.2, 6.0 Hz, 2H), 7.63 (d, *J* = 7.6 Hz, 2H), 7.39 – 7.27 (m, 5H), 7.15 (d, *J* = 7.8 Hz, 2H), 7.08 (t, *J* = 8.2 Hz, 2H), 4.85 (d, *J* = 15.1 Hz, 1H), 4.20 (d, *J* = 15.1 Hz, 1H), 3.97 (d, *J* = 15.1 Hz, 1H), 3.86 (d, *J* = 15.1

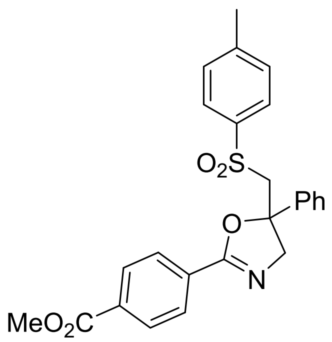
Hz, 1H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8 (d, J = 252.3 Hz), 161.4 (s), 144.5, 142.3, 137.4, 130.5 (d, J = 8.9 Hz), 129.6, 128.8, 128.2, 128.0, 124.4, 123.3 (d, J = 3.2 Hz), 115.4 (d, J = 22.0 Hz), 85.3, 66.6, 64.2, 21.5. ^{19}F NMR (376 MHz, $CDCl_3$) δ -107.59. HRMS (ESI) m/z calcd for $C_{23}H_{20}FNO_3S$ $[M+Na]^+$ 432.1040, found 432.1043.

2-(4-Bromophenyl)-5-phenyl-5-(tosylmethyl)-4,5-dihydrooxazole (3fa)



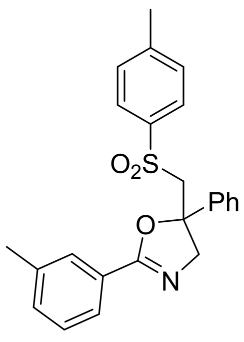
White solid. 60.3 mg, Yield: 64%, mp 186-187 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J = 8.0 Hz, 4H), 7.53 (d, J = 8.0 Hz, 2H), 7.39 – 7.27 (m, 5H), 7.14 (d, J = 7.9 Hz, 2H), 4.87 (d, J = 15.2 Hz, 1H), 4.20 (d, J = 15.2 Hz, 1H), 3.97 (d, J = 15.1 Hz, 1H), 3.85 (d, J = 15.1 Hz, 1H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.5, 144.6, 142.3, 137.3, 131.5, 129.8, 129.6, 128.9, 128.2, 128.0, 126.3, 126.0, 124.3, 85.4, 66.5, 64.2, 21.5. HRMS (ESI) m/z calcd for $C_{23}H_{20}BrNO_3S$ $[M+H]^+$ 470.0420, found 470.0423.

Methyl 4-(5-phenyl-5-(tosylmethyl)-4,5-dihydrooxazol-2-yl)benzoate (3ga)



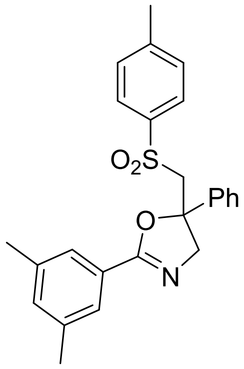
White solid. 53.9 mg, Yield: 60%, mp 108-109 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, J = 7.8 Hz, 2H), 7.83 (d, J = 7.9 Hz, 2H), 7.63 (d, J = 7.7 Hz, 2H), 7.39 – 7.27 (m, 5H), 7.14 (d, J = 7.5 Hz, 2H), 4.92 (d, J = 15.4 Hz, 1H), 4.25 (d, J = 15.4 Hz, 1H), 4.10 – 3.78 (m, 5H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 161.5, 144.6, 142.2, 137.2, 132.7, 131.0, 129.7, 129.4, 128.9, 128.3, 128.2, 128.0, 124.3, 85.5, 66.5, 64.2, 52.5, 21.5. HRMS (ESI) m/z calcd for $C_{25}H_{23}NO_5S$ $[M+Na]^+$ 472.1189, found 472.1191.

5-Phenyl-2-(m-tolyl)-5-(tosylmethyl)-4,5-dihydrooxazole (3ha)



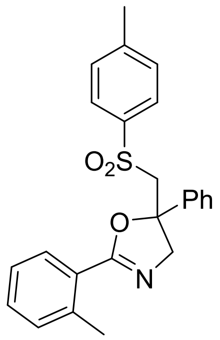
White solid. 59.2 mg, Yield: 73%, mp 172-174 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.7 Hz, 2H), 7.59 (s, 1H), 7.55 (d, *J* = 7.3 Hz, 1H), 7.40 – 7.25 (m, 7H), 7.14 (d, *J* = 7.8 Hz, 2H), 4.86 (d, *J* = 15.1 Hz, 1H), 4.21 (d, *J* = 15.1 Hz, 1H), 3.99 (d, *J* = 15.1 Hz, 1H), 3.88 (d, *J* = 15.2 Hz, 1H), 2.40 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.5, 144.4, 142.5, 138.0, 137.3, 132.4, 129.6, 128.8, 128.8, 128.1, 128.1, 126.8, 125.4, 124.4, 85.0, 66.6, 64.2, 21.5, 21.3. HRMS (ESI) *m/z* calcd for $C_{24}H_{23}NO_3S$ $[M+Na]^+$ 428.1291, found 428.1293.

2-(3,5-dimethylphenyl)-5-phenyl-5-(tosylmethyl)-4,5-dihydrooxazole (3ia)



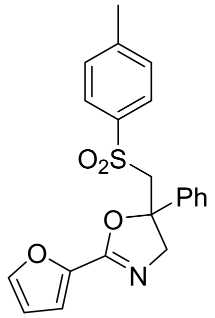
White solid. 62.0 mg, Yield: 74%, mp 178-180 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.7 Hz, 2H), 7.39 (s, 2H), 7.37 – 7.26 (m, 5H), 7.15 (d, *J* = 8.4 Hz, 3H), 4.85 (d, *J* = 15.0 Hz, 1H), 4.20 (d, *J* = 15.0 Hz, 1H), 4.00 (d, *J* = 15.2 Hz, 1H), 3.89 (d, *J* = 15.2 Hz, 1H), 2.36 (s, 6H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.6, 144.4, 142.5, 137.8, 137.4, 133.3, 129.6, 128.8, 128.1, 126.7, 126.0, 124.4, 84.9, 66.5, 64.2, 21.5, 21.2. HRMS (ESI) *m/z* calcd for $C_{25}H_{25}NO_3S$ $[M+Na]^+$ 442.1447, found 442.1450.

5-Phenyl-2-(o-tolyl)-5-(tosylmethyl)-4,5-dihydrooxazole (3ja)



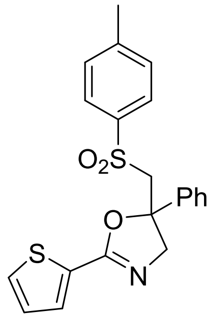
White solid. 57.5 mg, Yield: 71%, mp 106-107 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.7 Hz, 3H), 7.41 – 7.24 (m, 7H), 7.20 (t, *J* = 7.4 Hz, 1H), 7.12 (d, *J* = 7.7 Hz, 2H), 4.86 (d, *J* = 15.1 Hz, 1H), 4.28 (d, *J* = 15.1 Hz, 1H), 3.97 (d, *J* = 15.1 Hz, 1H), 3.86 (d, *J* = 15.0 Hz, 1H), 2.61 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4, 144.4, 142.4, 139.4, 137.4, 131.3, 130.8, 130.0, 129.6, 128.8, 128.1, 127.9, 126.0, 125.4, 124.6, 84.0, 67.3, 64.4, 22.3, 21.6. HRMS (ESI) *m/z* calcd for $C_{24}H_{23}NO_3S$ $[M+Na]^+$ 428.1291, found 428.1292.

2-(Furan-2-yl)-5-phenyl-5-(tosylmethyl)-4,5-dihydrooxazole (3ka)



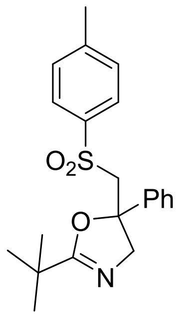
White solid. 39.6 mg, Yield: 52%, mp 136-137 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, J = 7.7 Hz, 2H), 7.55 (s, 1H), 7.36 – 7.27 (m, 5H), 7.19 (d, J = 7.7 Hz, 2H), 6.77 (d, J = 2.4 Hz, 1H), 6.49 (d, J = 1.2 Hz, 1H), 4.88 (d, J = 15.2 Hz, 1H), 4.22 (d, J = 15.2 Hz, 1H), 3.96 (d, J = 15.1 Hz, 1H), 3.85 (d, J = 15.2 Hz, 1H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.7, 145.5, 144.6, 142.2, 141.9, 137.2, 129.6, 128.8, 128.3, 128.1, 124.5, 114.7, 111.5, 85.5, 66.1, 64.2, 21.6. HRMS (ESI) *m/z* calcd for $C_{21}H_{19}NO_4S$ $[M+Na]^+$ 404.0927, found 404.0929.

5-phenyl-2-(thiophen-2-yl)-5-(tosylmethyl)-4,5-dihydrooxazole (3la)



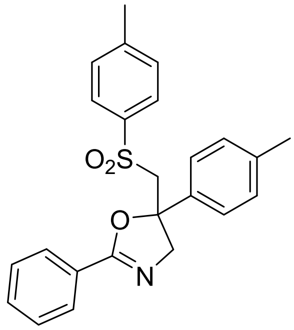
White solid. 44.5 mg, Yield: 56%, mp 134-136 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, J = 7.8 Hz, 2H), 7.48 (d, J = 3.7 Hz, 1H), 7.39 – 7.26 (m, 6H), 7.17 (d, J = 7.8 Hz, 2H), 7.06 (s, 1H), 4.86 (d, J = 15.0 Hz, 1H), 4.20 (d, J = 15.0 Hz, 1H), 3.98 (d, J = 15.1 Hz, 1H), 3.87 (d, J = 15.2 Hz, 1H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.1, 144.6, 142.2, 137.2, 130.6, 130.3, 129.6, 129.6, 128.8, 128.2, 128.1, 127.4, 124.4, 85.6, 66.3, 64.2, 21.6. HRMS (ESI) *m/z* calcd for $C_{21}H_{19}NO_3S_2$ $[M+Na]^+$ 420.0699, found 420.0701.

2-(Tert-butyl)-5-phenyl-5-(tosylmethyl)-4,5-dihydrooxazole (3ma)



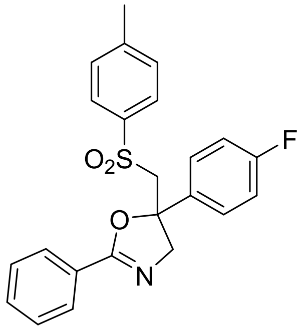
White solid. 37.1 mg, Yield: 50%, mp 102-103 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, J = 7.6 Hz, 2H), 7.34 – 7.16 (m, 7H), 4.38 (d, J = 14.5 Hz, 1H), 4.02 (d, J = 14.5 Hz, 1H), 3.82 (d, J = 14.7 Hz, 1H), 3.72 (d, J = 14.8 Hz, 1H), 2.41 (s, 3H), 1.23 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.9, 144.5, 142.0, 137.7, 129.6, 128.6, 128.0, 127.9, 124.7, 84.8, 67.3, 64.9, 33.3, 27.6, 21.6. HRMS (ESI) *m/z* calcd for $C_{21}H_{25}NO_3S$ $[M+Na]^+$ 394.1447, found 394.14450.

2-Phenyl-5-(*p*-tolyl)-5-(tosylmethyl)-4,5-dihydrooxazole (3na)



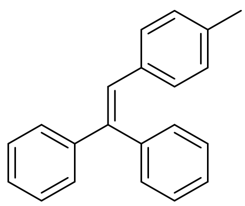
White solid. 56.7 mg, Yield: 70%, mp 148-150 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 7.5 Hz, 2H), 7.61 (d, *J* = 7.6 Hz, 2H), 7.47 (t, *J* = 7.3 Hz, 1H), 7.36 (t, *J* = 7.3 Hz, 2H), 7.18 (d, *J* = 7.5 Hz, 2H), 7.12 (d, *J* = 8.3 Hz, 4H), 4.80 (d, *J* = 15.0 Hz, 1H), 4.18 (d, *J* = 15.1 Hz, 1H), 3.94 (d, *J* = 15.1 Hz, 1H), 3.84 (d, *J* = 15.1 Hz, 1H), 2.32 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.3, 144.4, 139.3, 138.0, 137.3, 131.5, 129.6, 129.4, 128.2, 128.2, 128.1, 127.0, 124.4, 85.1, 66.6, 64.3, 21.5, 21.1. HRMS (ESI) *m/z* calcd for $C_{24}H_{23}NO_3S$ $[M+Na]^+$ 428.1291, found 428.1292.

5-(4-Fluorophenyl)-2-phenyl-5-(tosylmethyl)-4,5-dihydrooxazole (3oa)



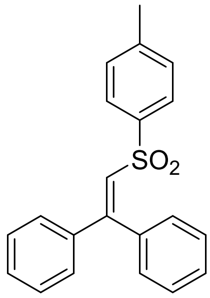
White solid. 58.5 mg, Yield: 74%, mp 133-134 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.4 Hz, 2H), 7.62 (d, *J* = 7.7 Hz, 2H), 7.50 (d, *J* = 7.2 Hz, 1H), 7.39 (t, *J* = 7.2 Hz, 2H), 7.35 – 7.26 (m, 2H), 7.16 (d, *J* = 7.6 Hz, 2H), 7.02 (t, *J* = 8.2 Hz, 2H), 4.79 (d, *J* = 15.1 Hz, 1H), 4.19 (d, *J* = 15.1 Hz, 1H), 3.95 (d, *J* = 15.0 Hz, 1H), 3.87 (d, *J* = 15.0 Hz, 1H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9 (d, *J* = 248.0 Hz), 162.2, 144.7, 137.9 (d, *J* = 3.1 Hz), 137.2, 131.7, 129.7, 128.3, 128.2, 128.0, 126.8, 126.5 (d, *J* = 8.3 Hz), 115.7 (d, *J* = 21.7 Hz), 84.8, 67.0, 64.3, 21.5. ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.72. HRMS (ESI) *m/z* calcd for $C_{23}H_{20}FNO_3S$ $[M+Na]^+$ 432.1040, found 432.1041.

(2-(*p*-Tolyl)ethene-1,1-diyl)dibenzene (4)



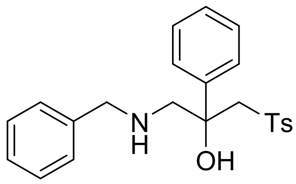
White solid. 9.7 mg, Yield: 18%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.21 (m, 10H), 6.99 – 6.86 (m, 5H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.6, 141.7, 140.6, 136.6, 134.5, 130.4, 129.5, 128.7, 128.7, 128.2, 128.1, 127.5, 127.4, 127.3, 21.2.

(2-Tosylethene-1,1-diyl)dibenzene (5)



White solid. 50.8 mg, Yield: 76%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.2 Hz, 2H), 7.39 – 7.33 (m, 6H), 7.24 – 7.12 (m, 6H), 7.03 (s, 1H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.8, 143.8, 139.2, 138.6, 135.6, 130.3, 129.8, 129.4, 129.0, 128.9, 128.6, 128.2, 127.8, 127.7, 21.6.

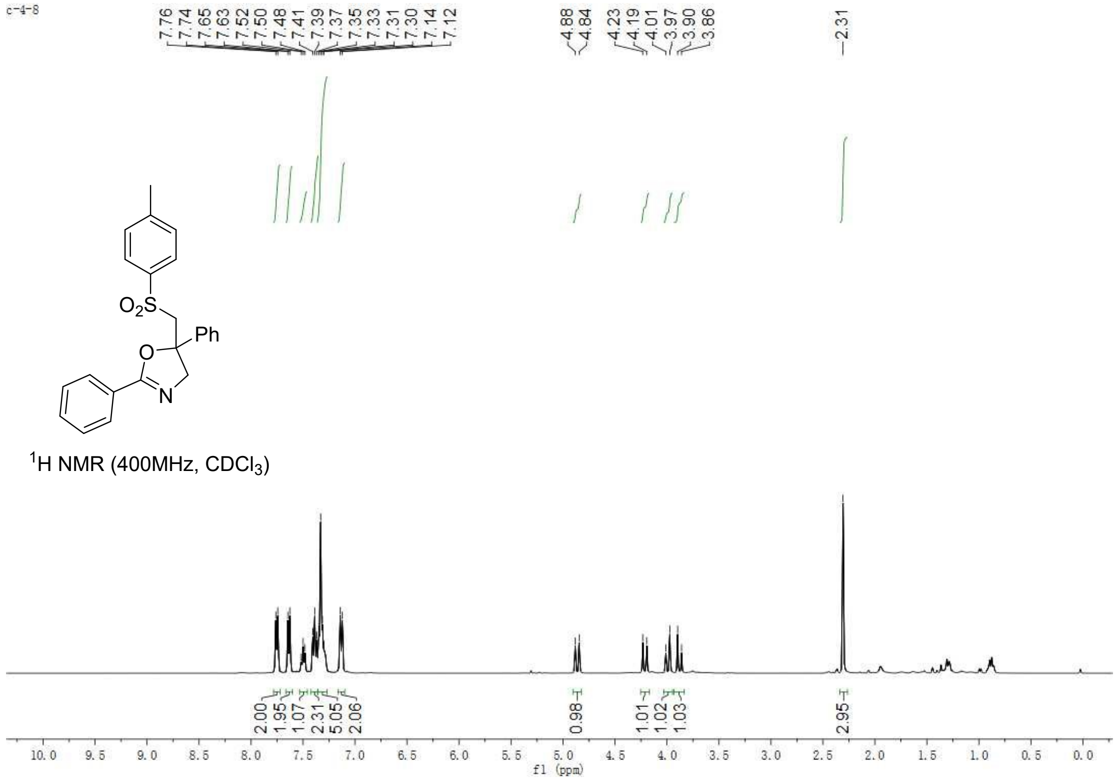
1-(Benzylamino)-2-phenyl-3-tosylpropan-2-ol (6)



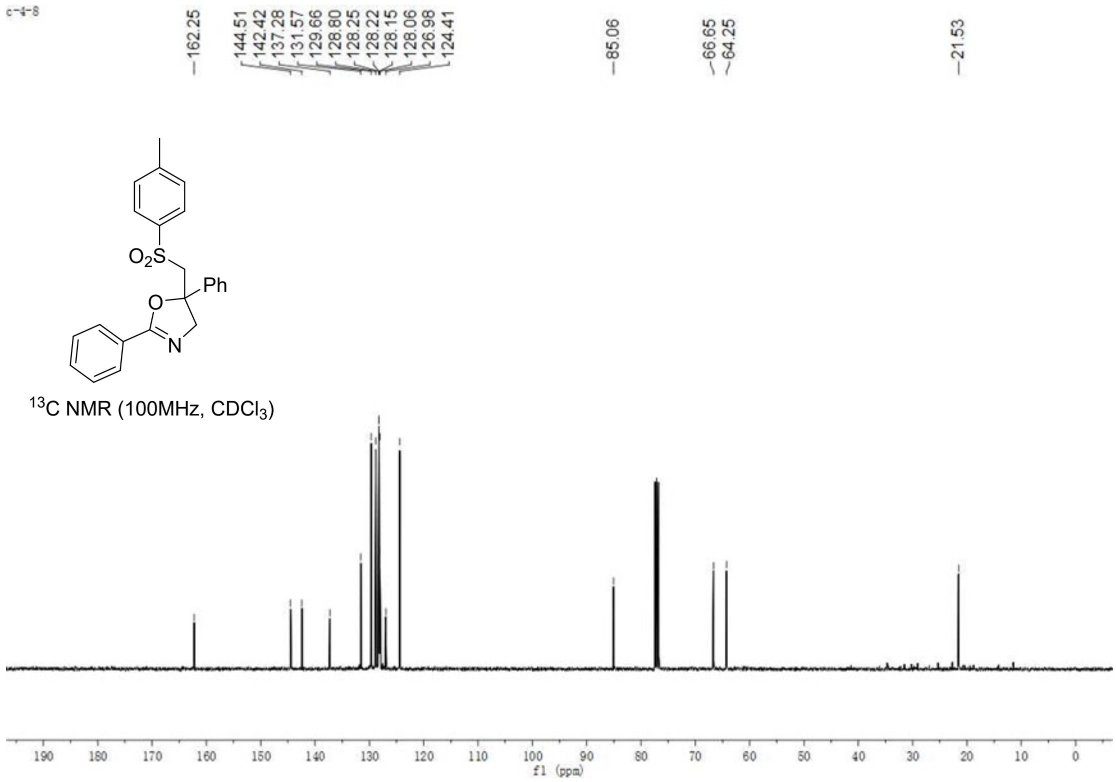
White solid. 71.1 mg, Yield: 90%, mp 151-153 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 7.8 Hz, 2H), 7.33 – 7.26 (m, 7H), 7.19 – 7.13 (m, 5H), 4.02 (d, *J* = 15.0 Hz, 1H), 3.85 – 3.68 (m, 3H), 3.02 – 2.95 (m, 2H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.2, 142.4, 139.9, 137.6, 129.5, 128.4, 128.2, 128.0, 127.7, 127.3, 127.1, 125.2, 74.6, 63.6, 58.9, 53.7, 21.6. HRMS (ESI) *m/z* calcd for $C_{23}H_{25}NO_3S$ $[M+H]^+$ 396.1628, found 396.1631.

9. Copies of the ^{1}H, ^{13}C and ^{19}F NMR Spectra

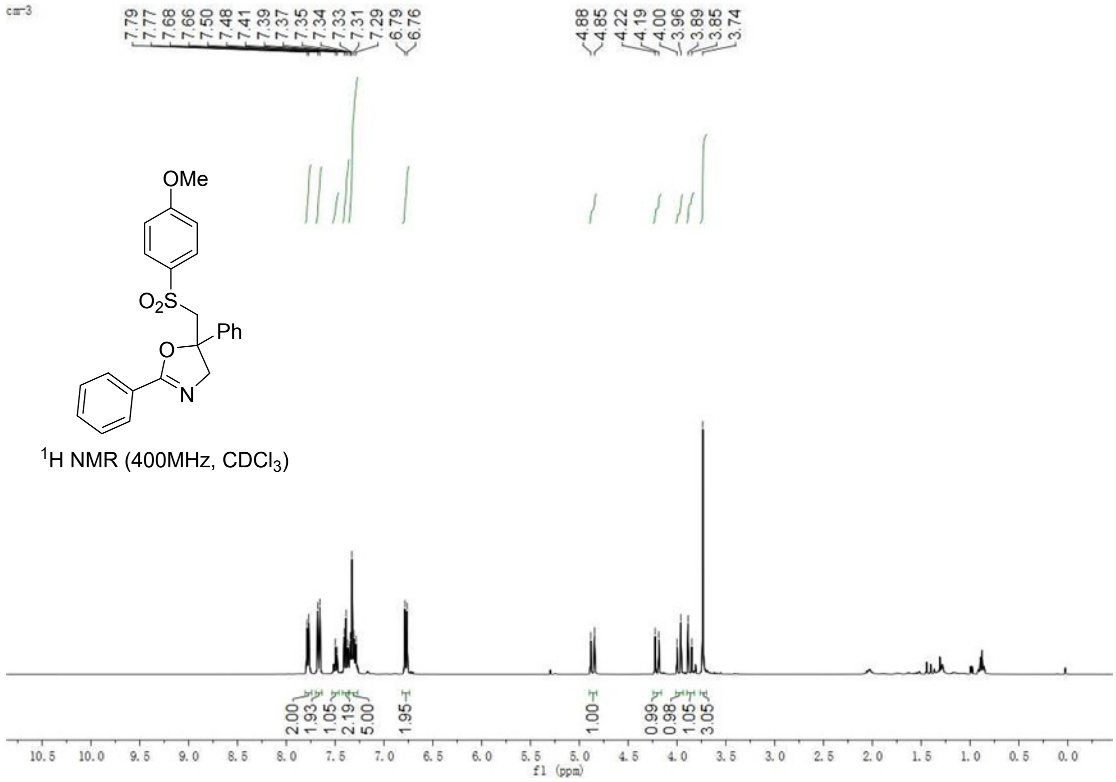
^{1}H NMR spectrum of **3aa**



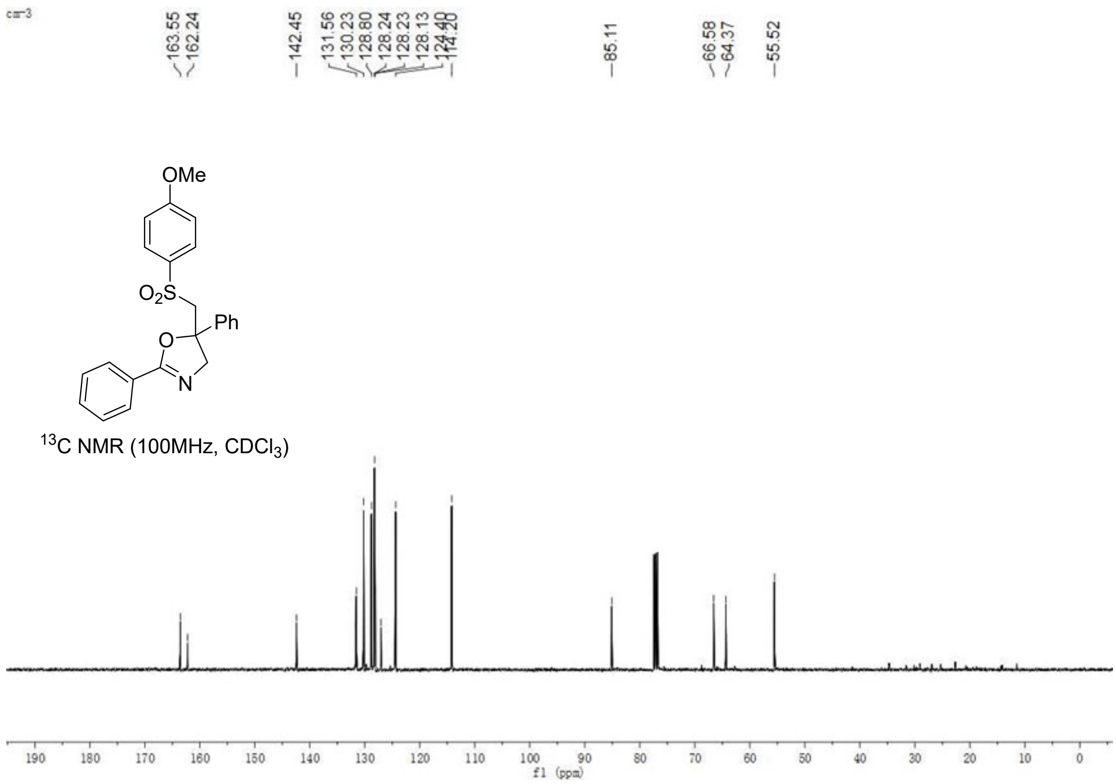
^{13}C NMR spectrum of **3aa**



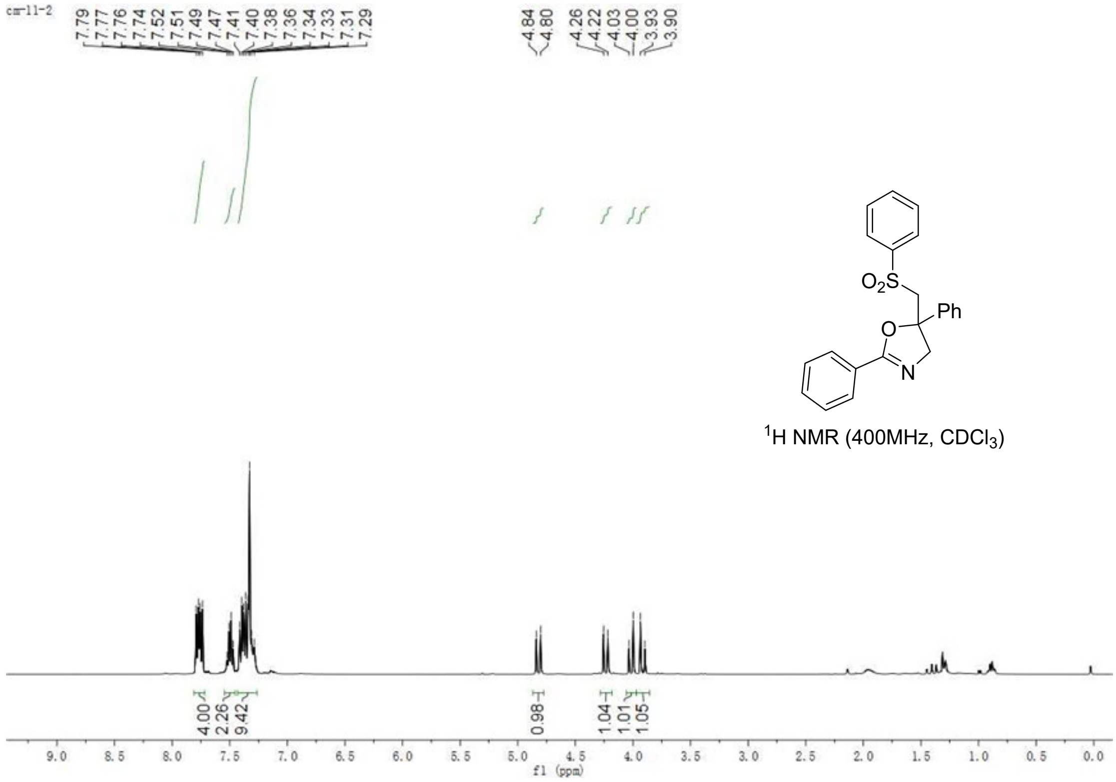
^{1}H NMR spectrum of **3ab**



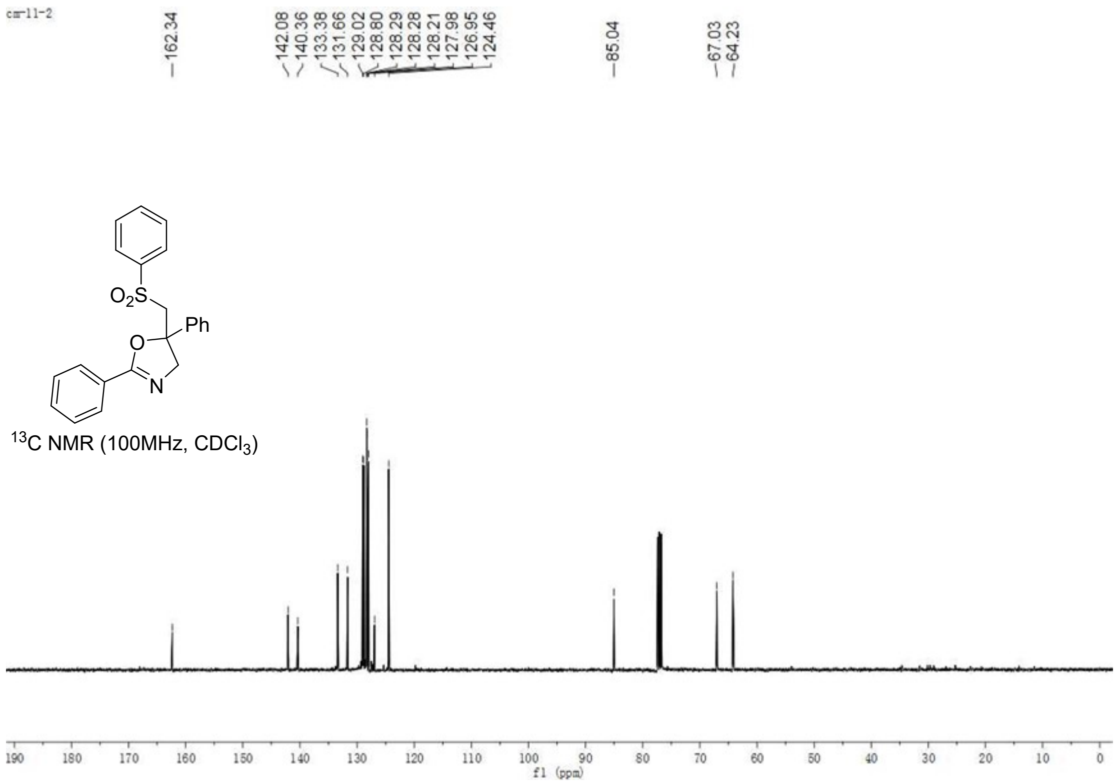
^{13}C NMR spectrum of **3ab**



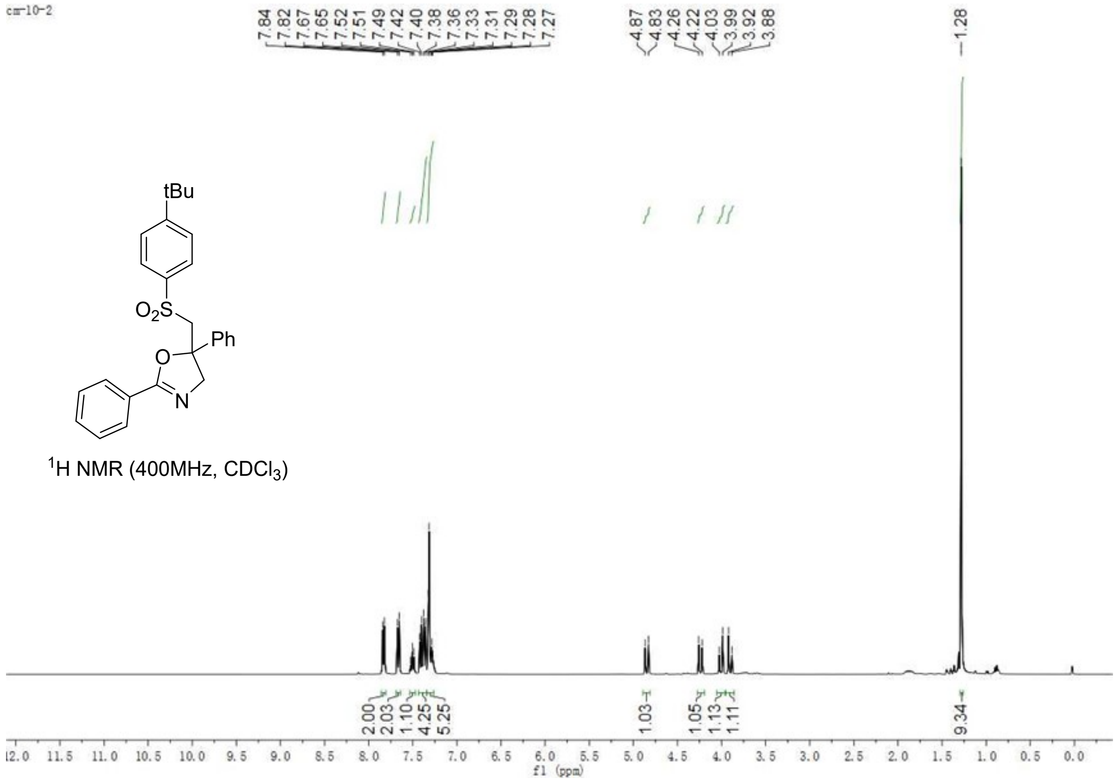
^{1}H NMR spectrum of **3ac**



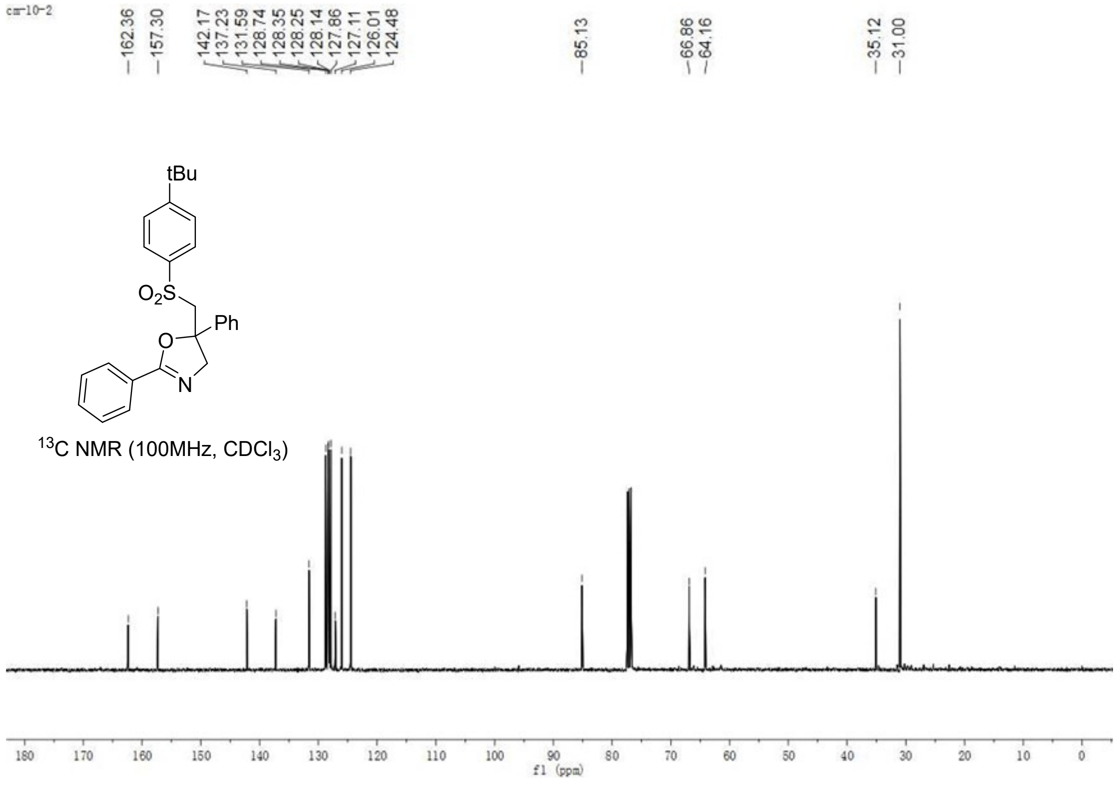
^{13}C NMR spectrum of **3ac**



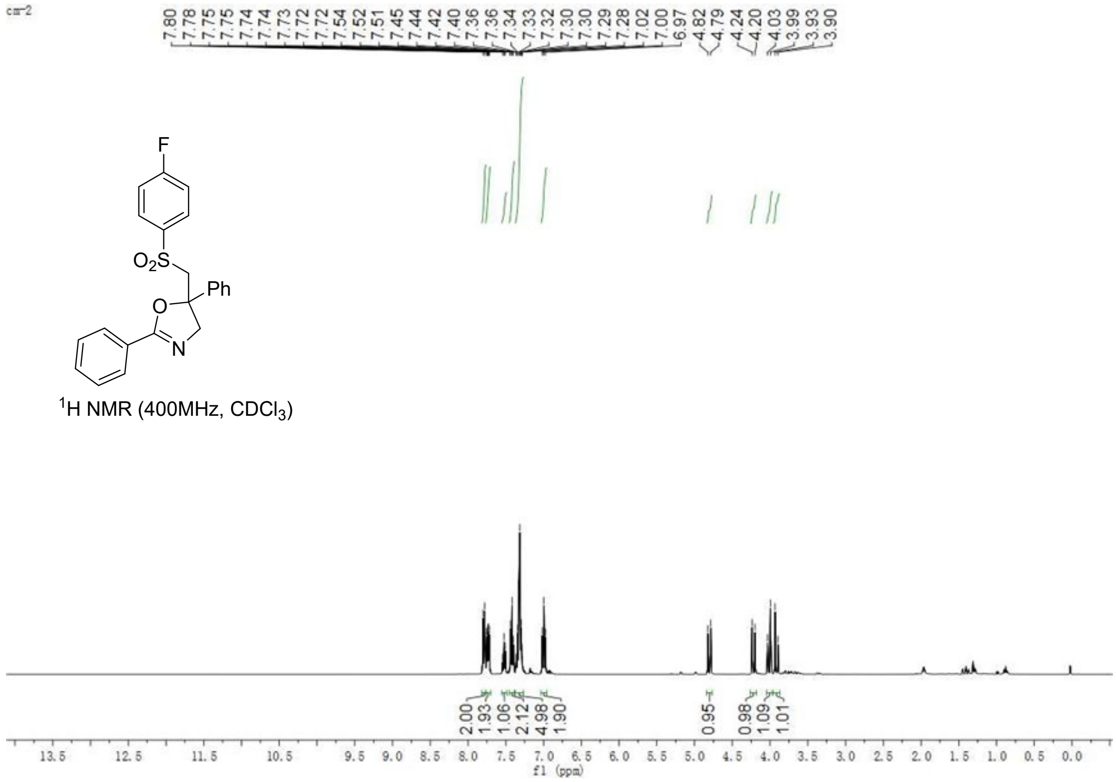
¹H NMR spectrum of **3ad**



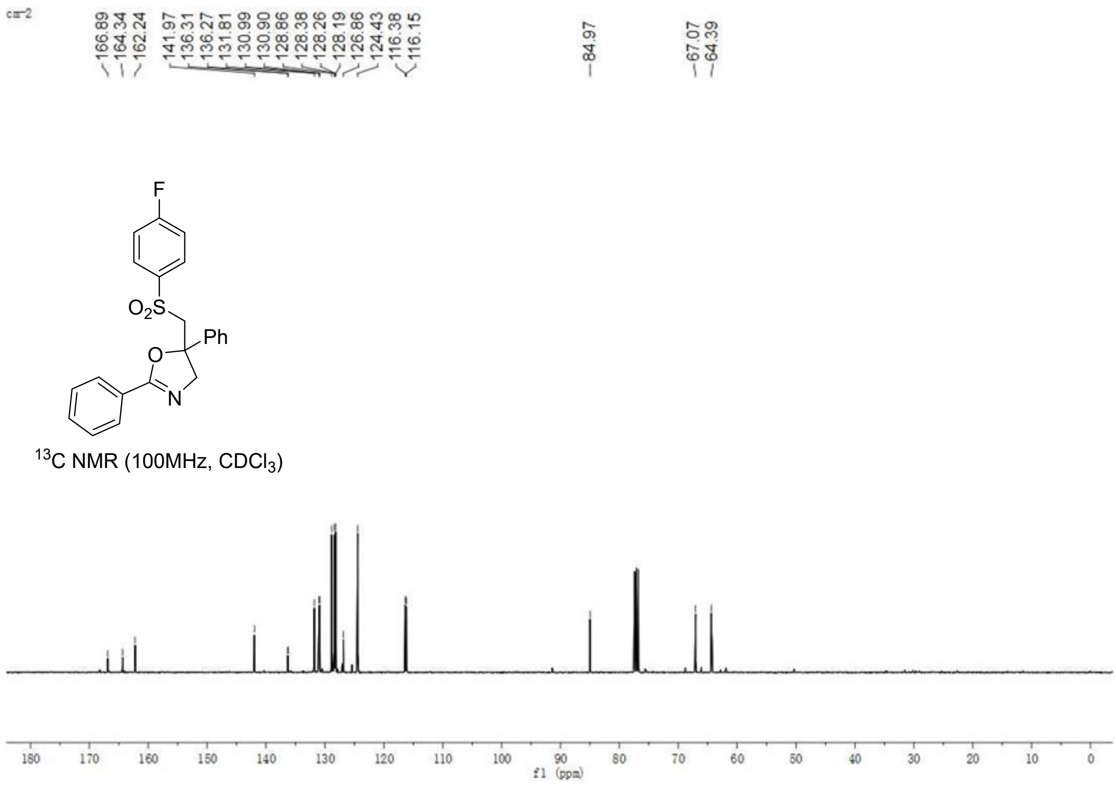
¹³C NMR spectrum of **3ad**



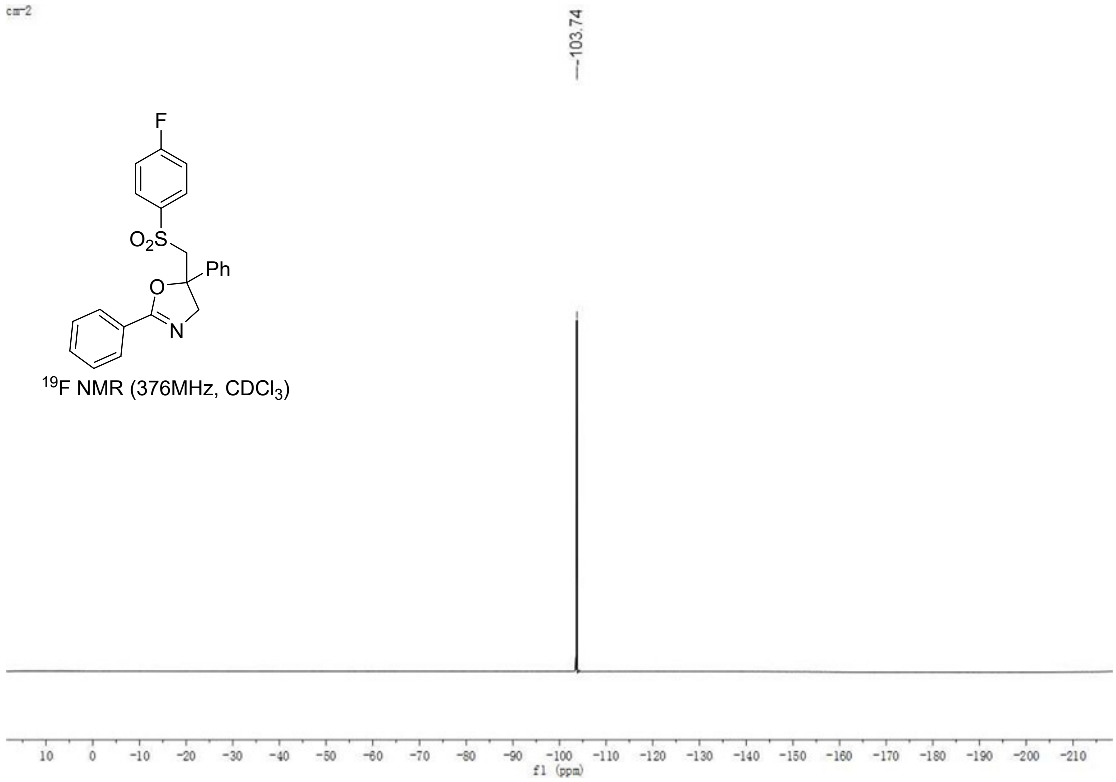
^{1}H NMR spectrum of **3ae**



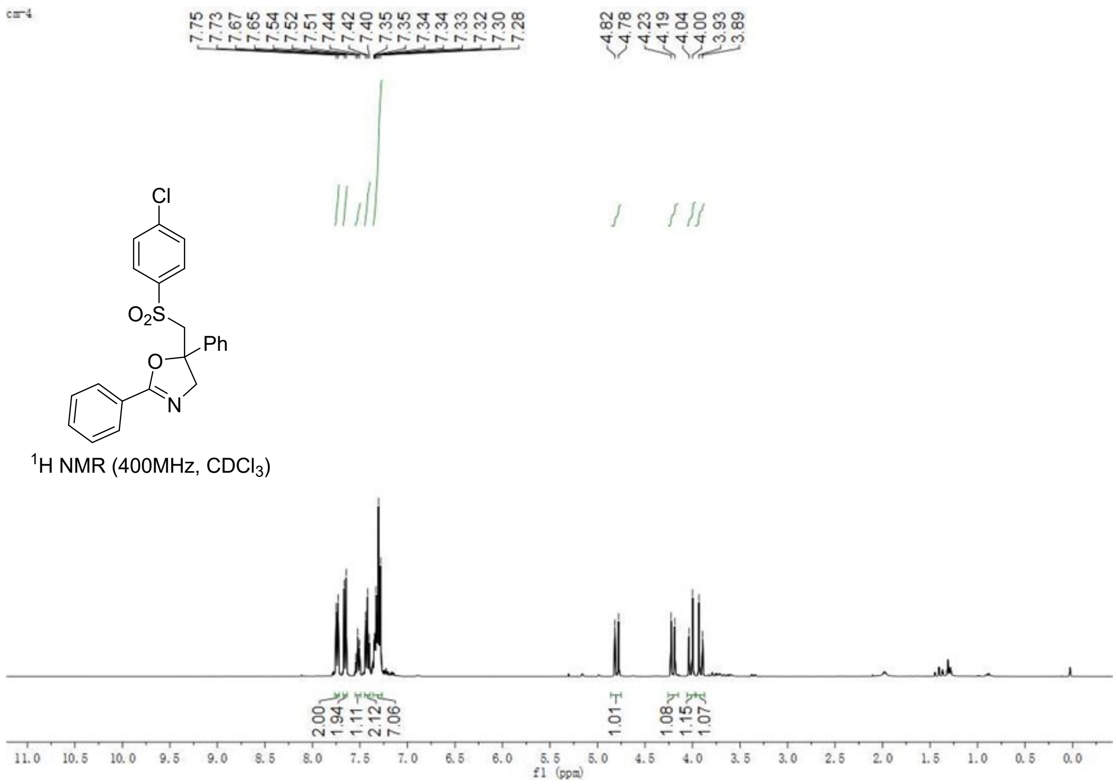
^{13}C NMR spectrum of **3ae**



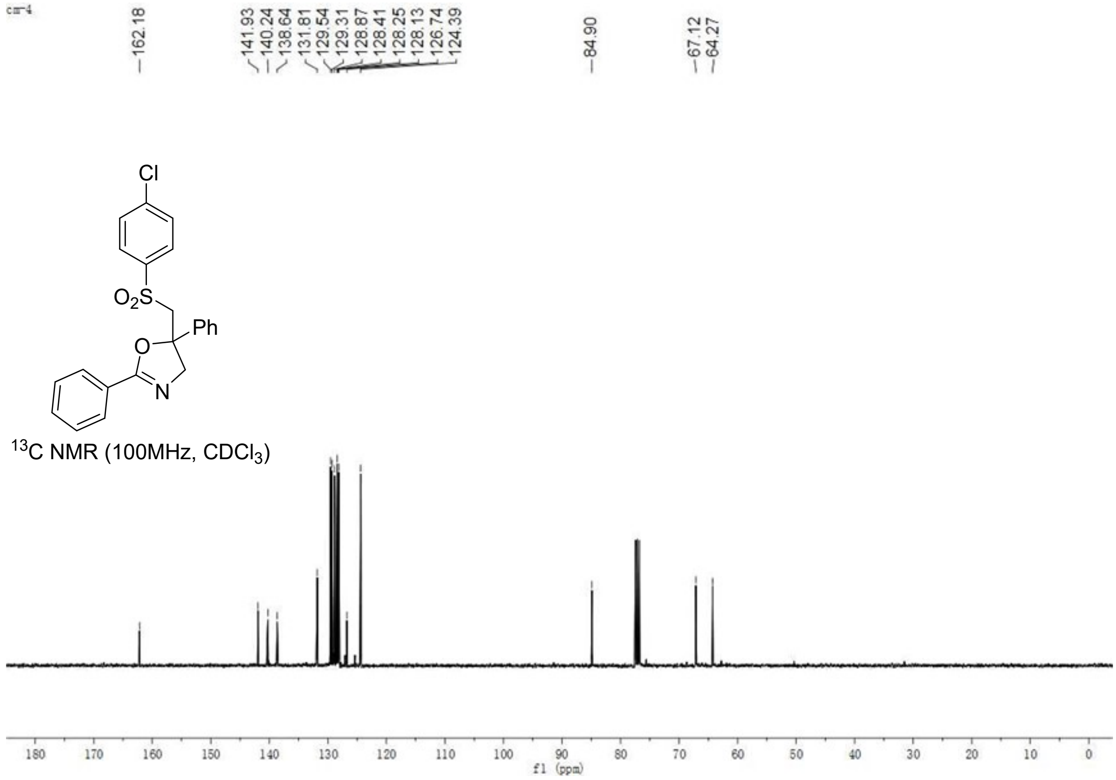
^{19}F NMR spectrum of **3ae**



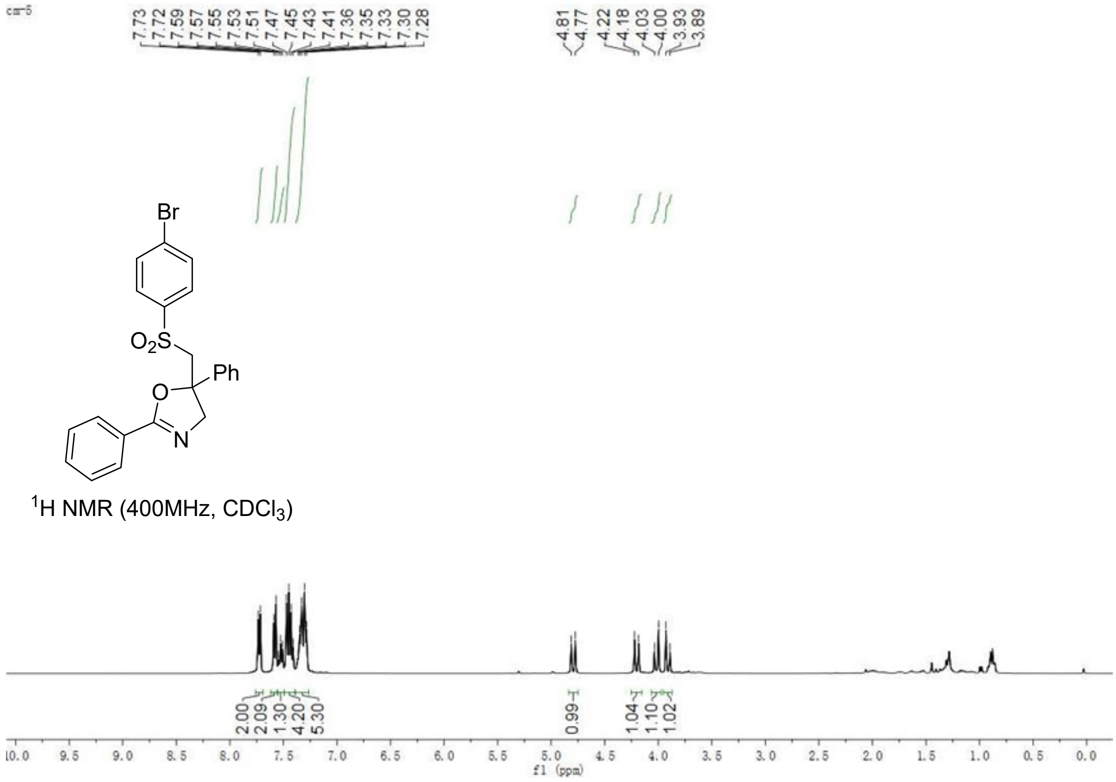
^{1}H NMR spectrum of **3af**



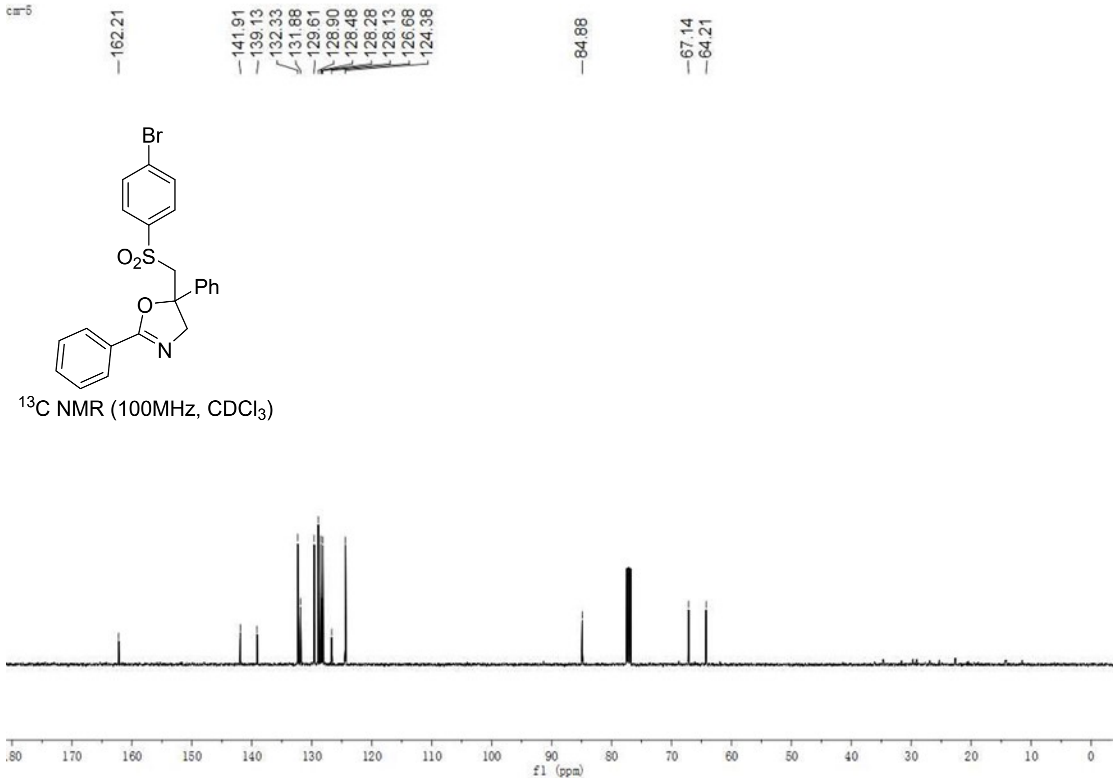
^{13}C NMR spectrum of **3af**



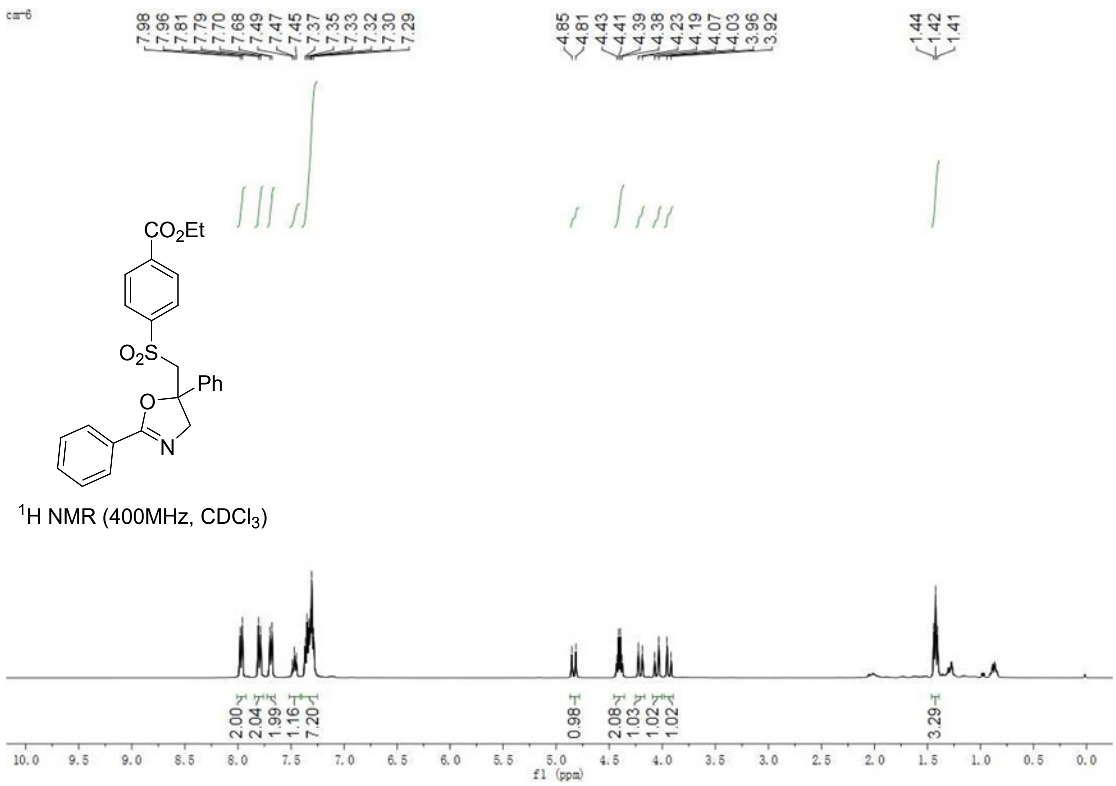
^{1}H NMR spectrum of **3ag**



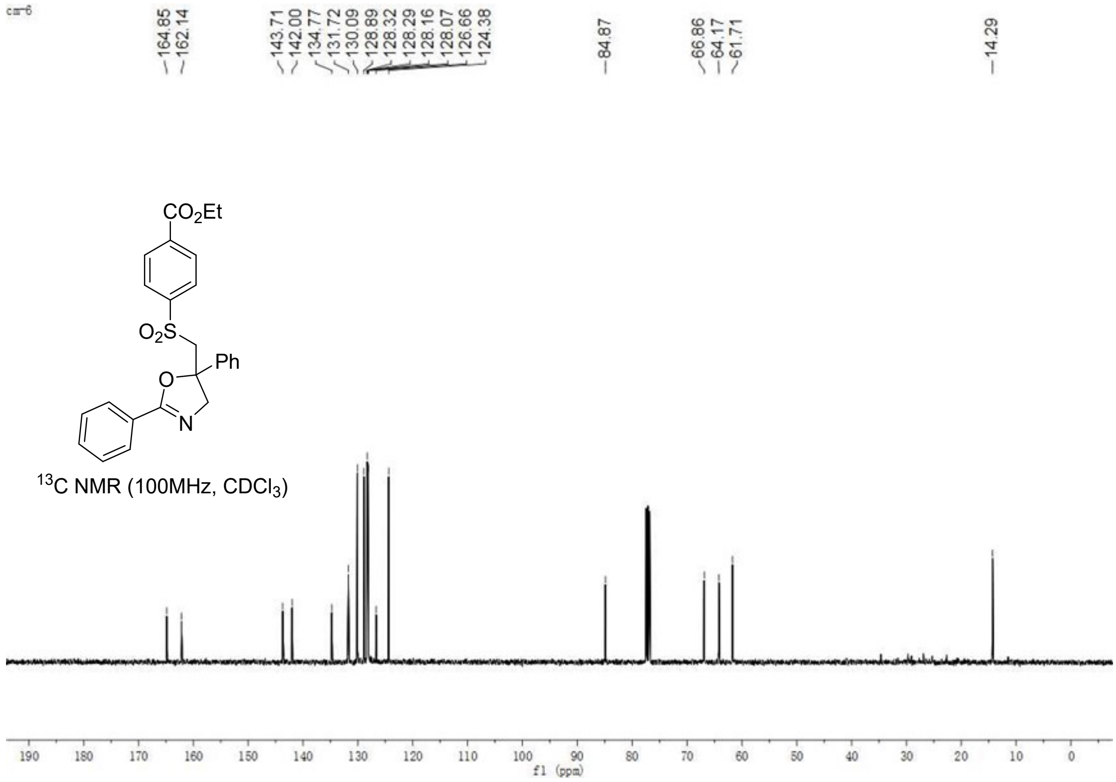
^{13}C NMR spectrum of **3ag**



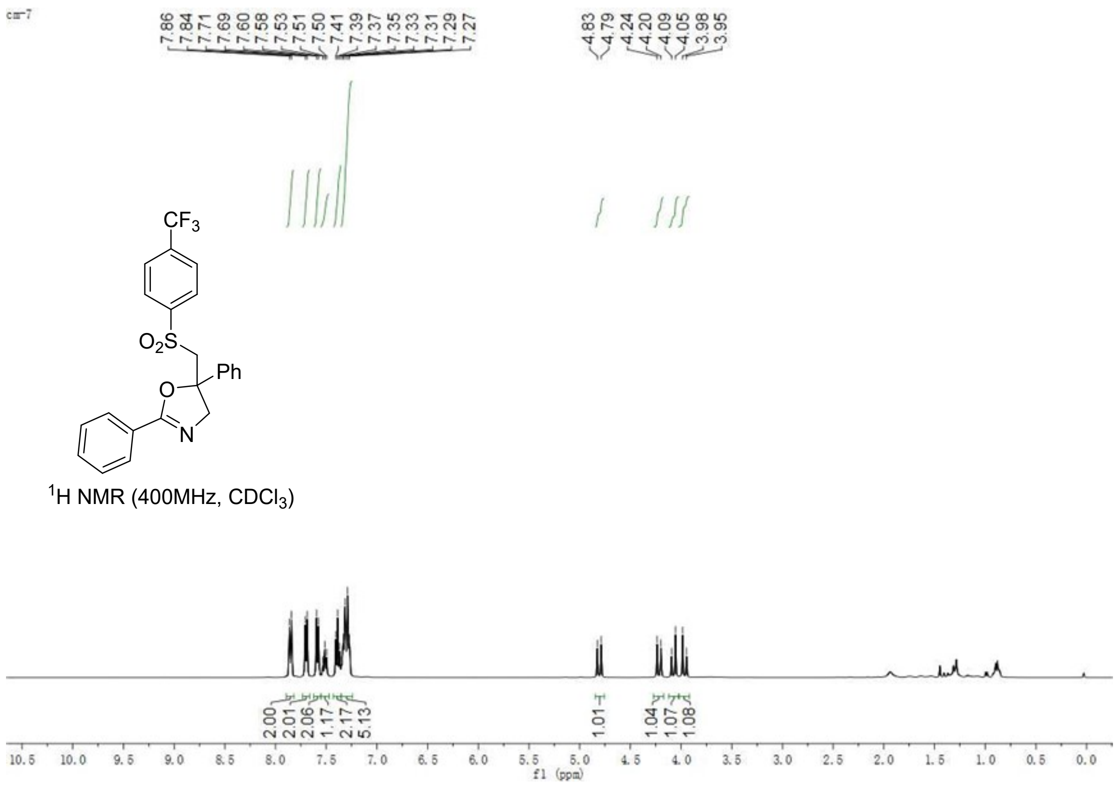
^{1}H NMR spectrum of **3ah**



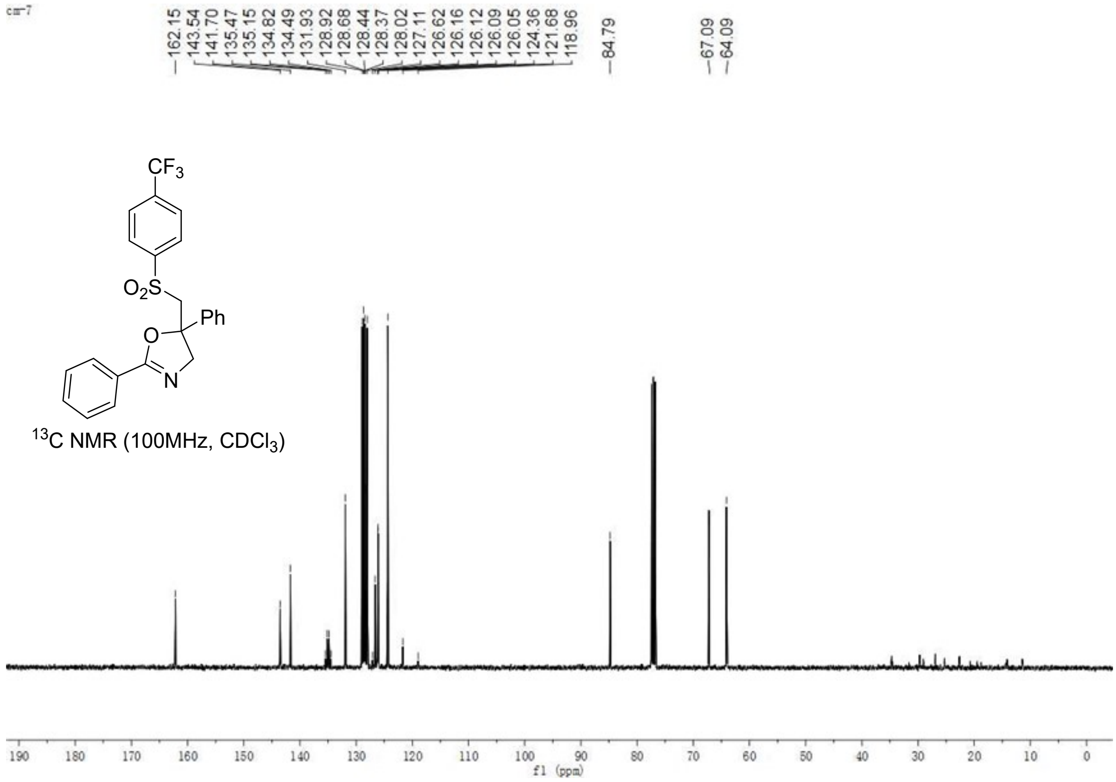
^{13}C NMR spectrum of **3ah**



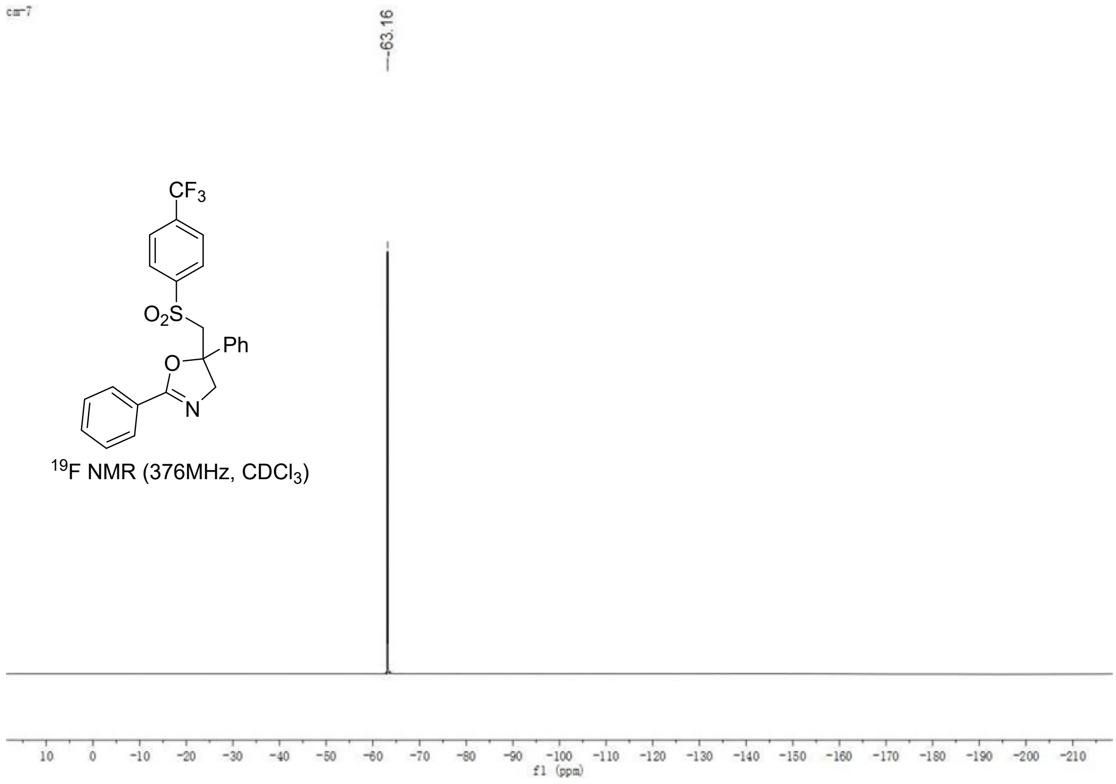
^{1}H NMR spectrum of **3ai**



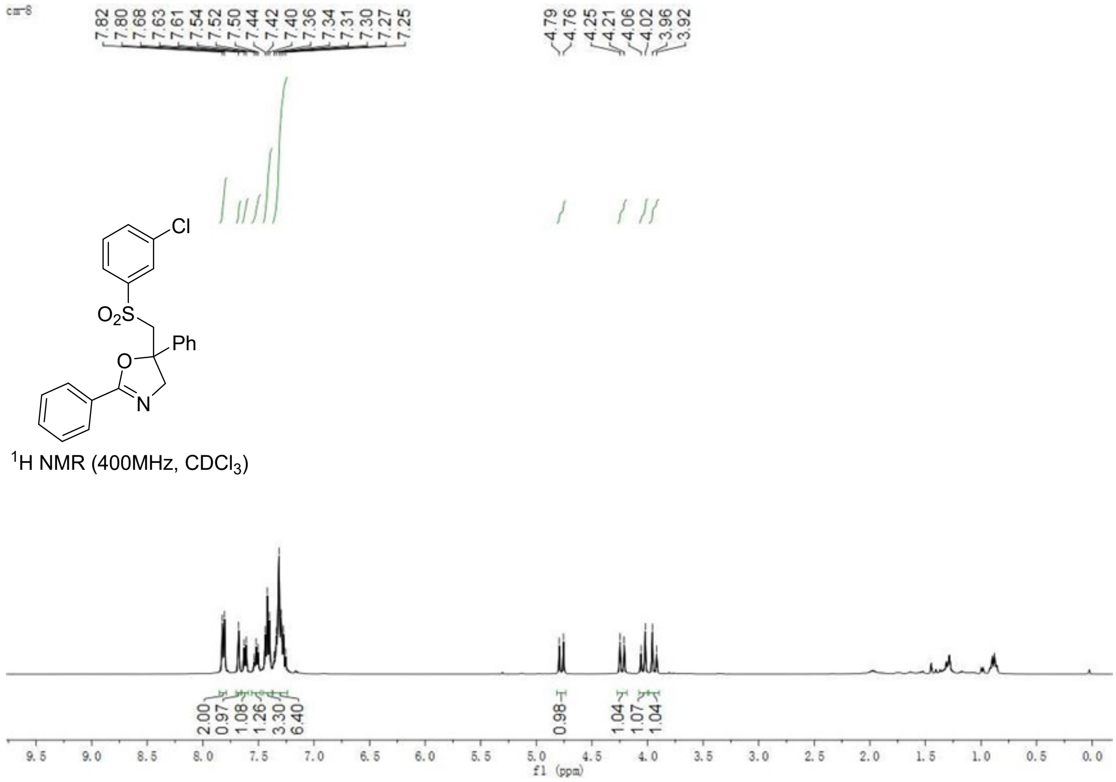
^{13}C NMR spectrum of **3ai**



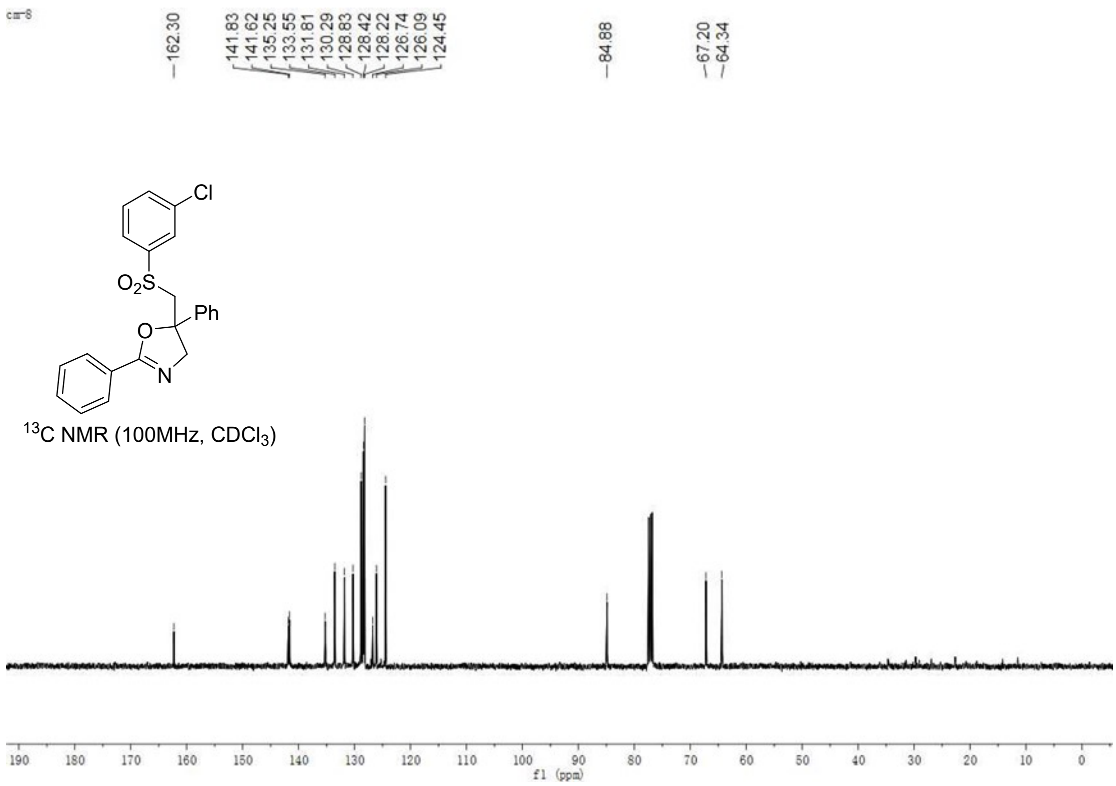
^{19}F NMR spectrum of **3ai**



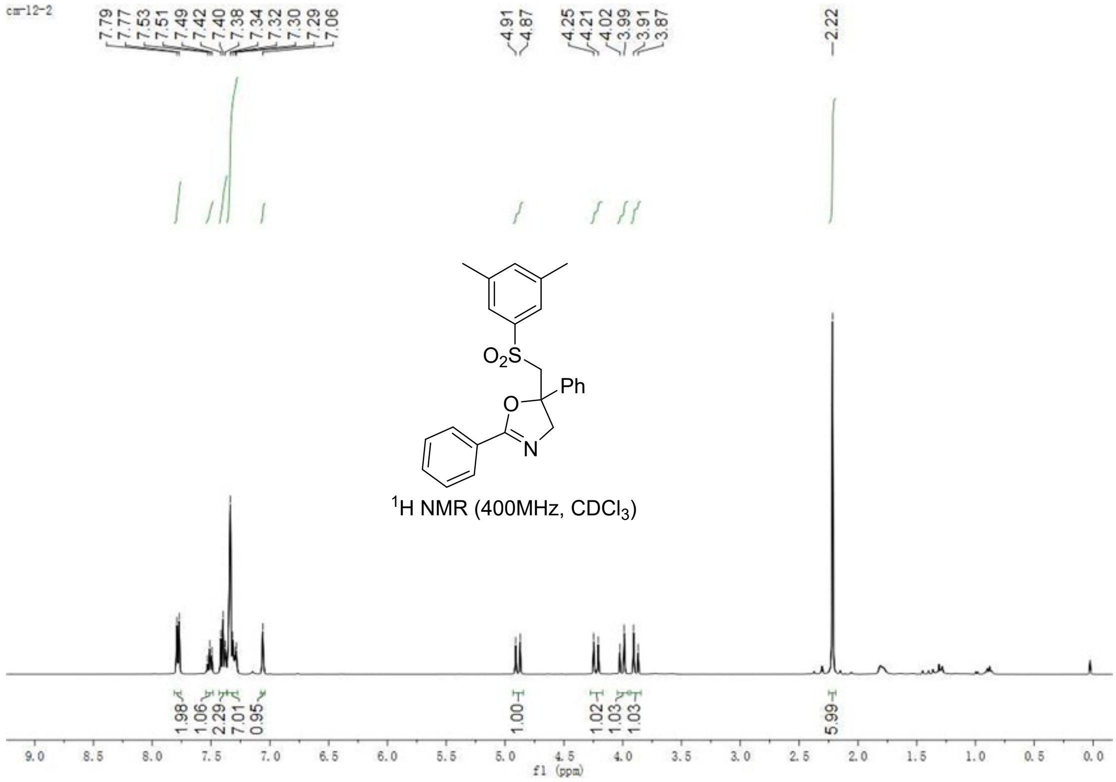
^{1}H NMR spectrum of **3aj**



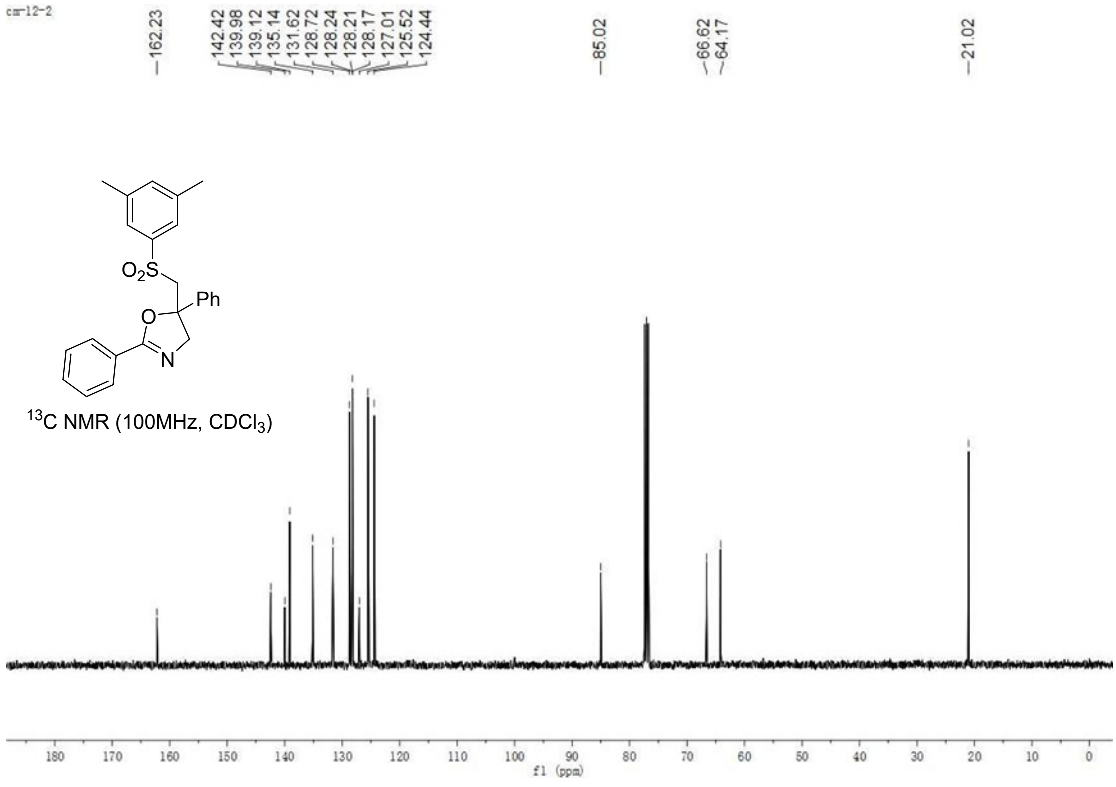
^{13}C NMR spectrum of **3aj**



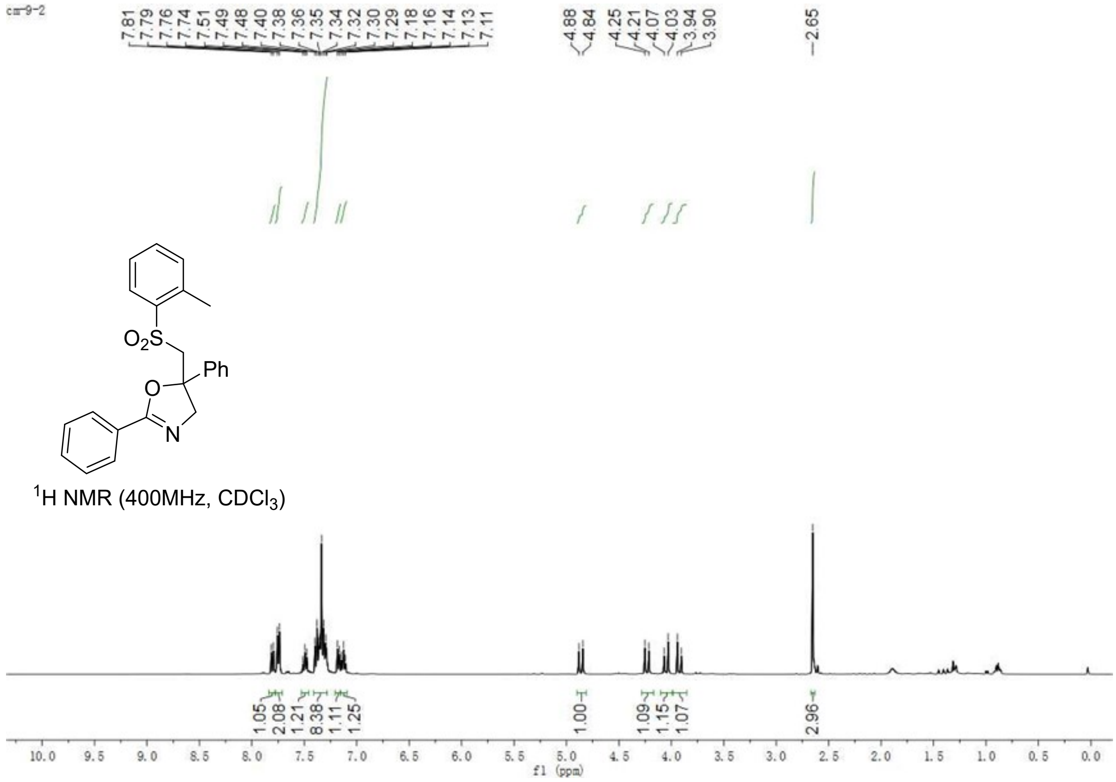
^{1}H NMR spectrum of **3ak**



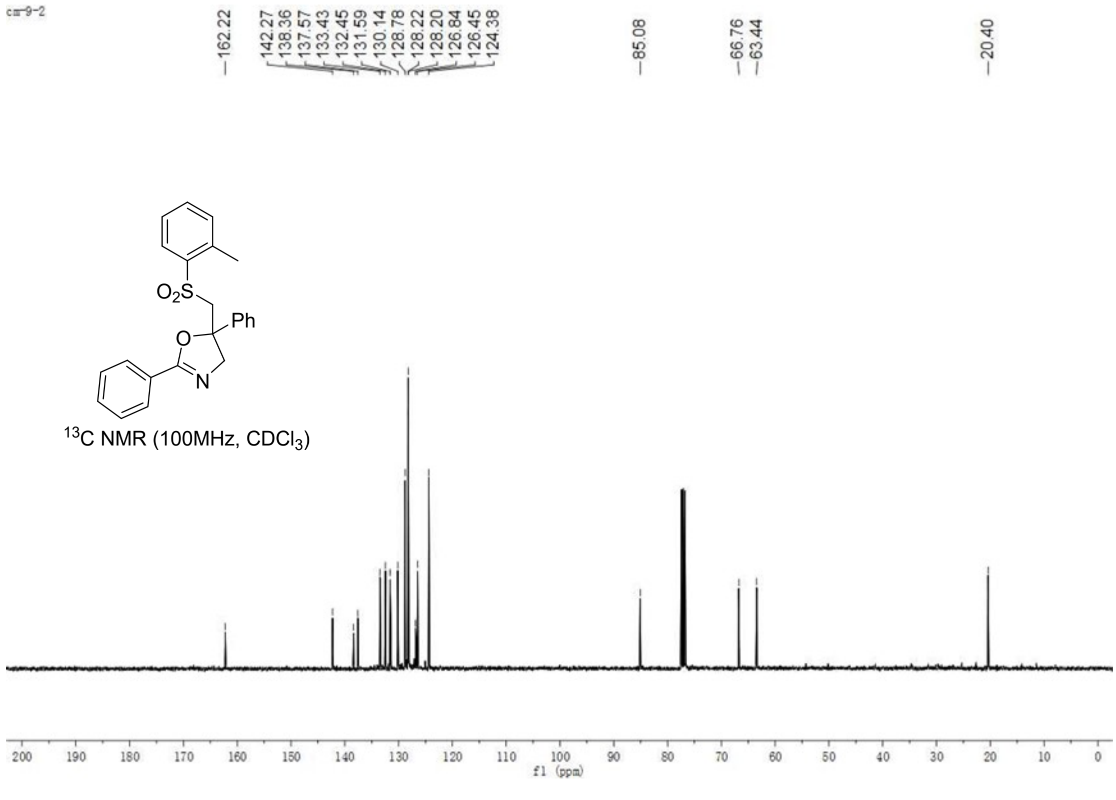
^{13}C NMR spectrum of **3ak**



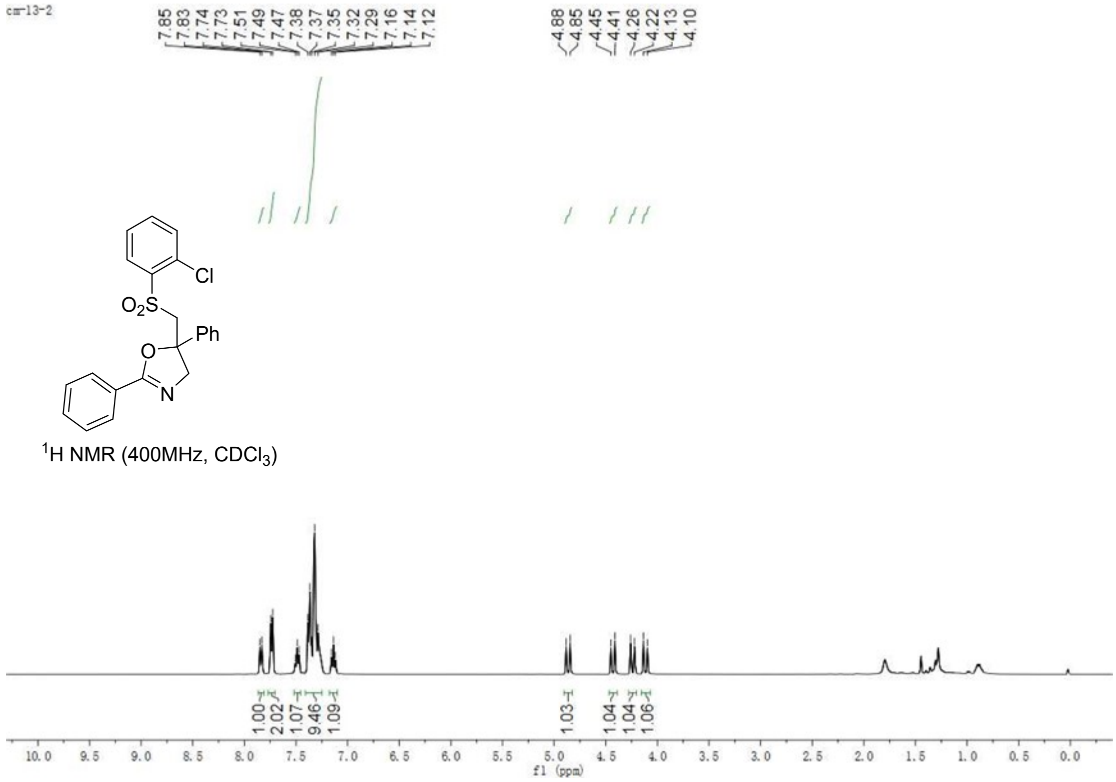
^{1}H NMR spectrum of **3al**



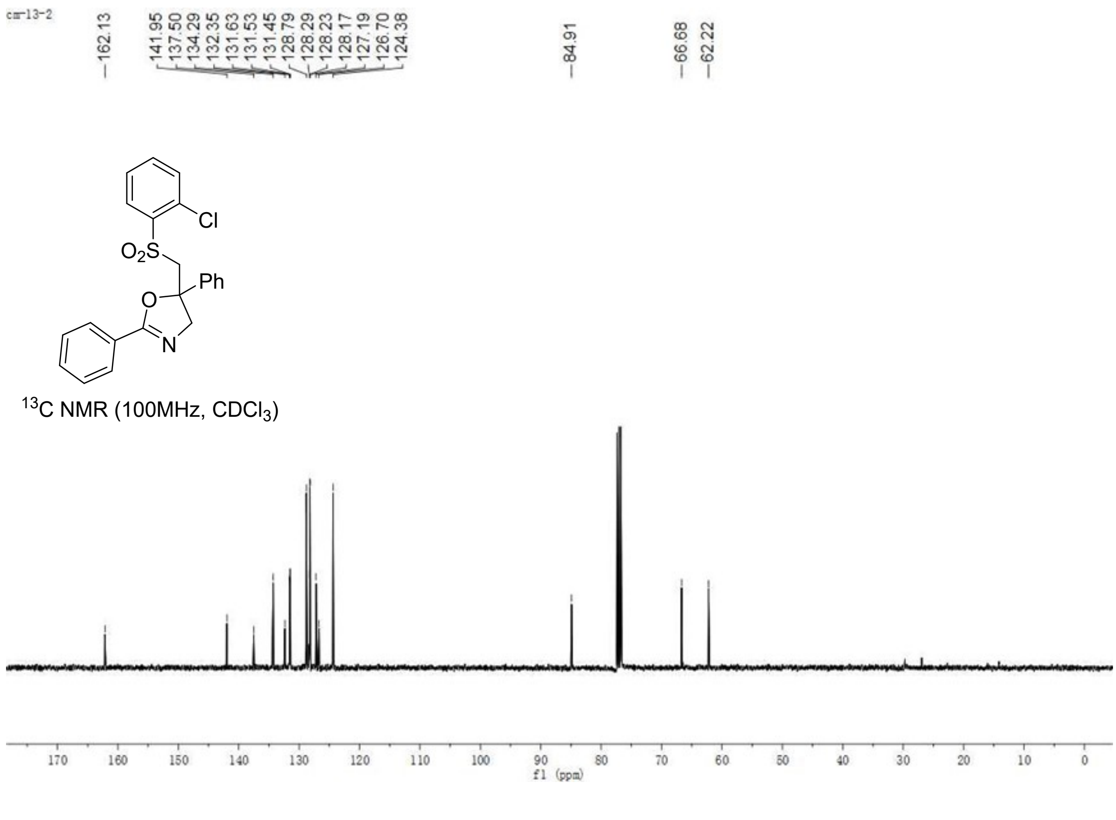
^{13}C NMR spectrum of **3al**



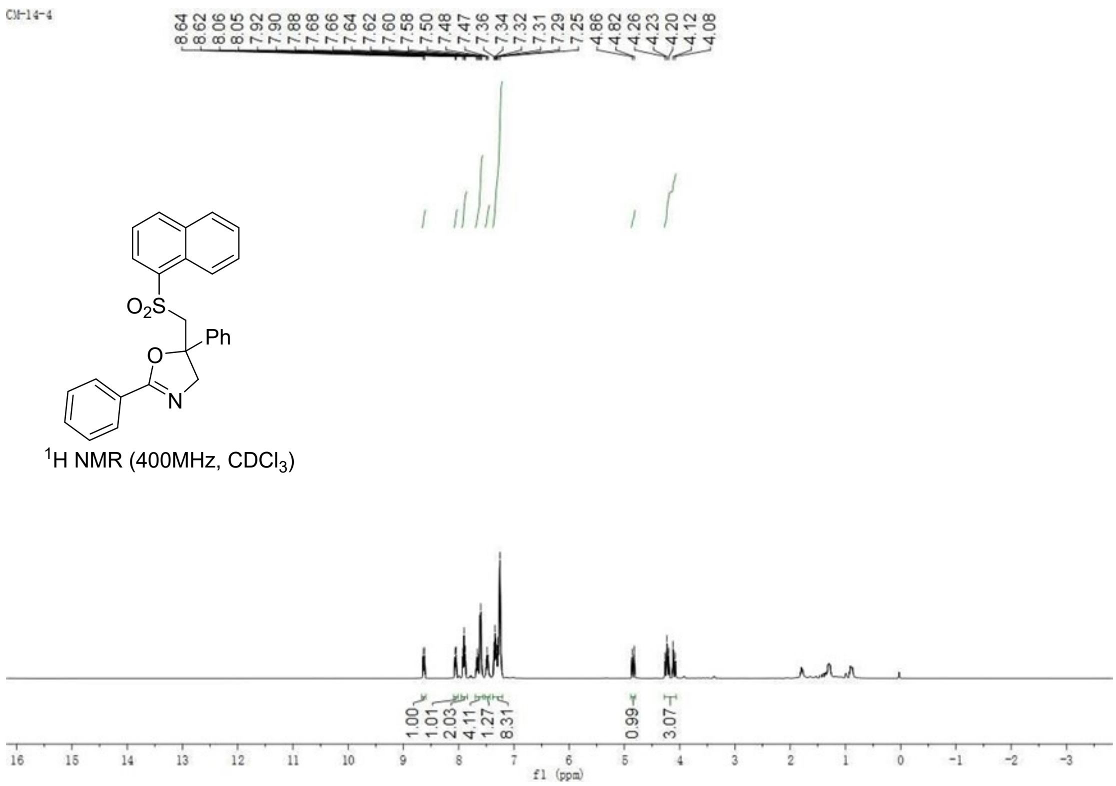
^{1}H NMR spectrum of **3am**



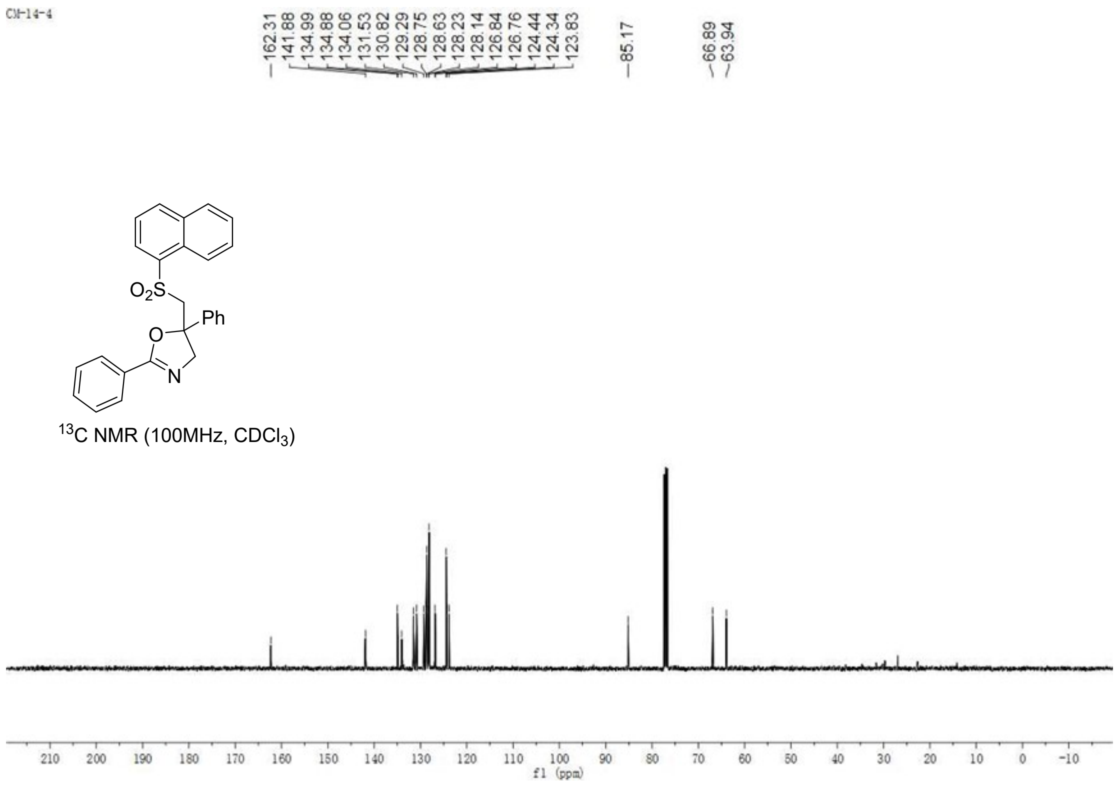
^{13}C NMR spectrum of **3am**



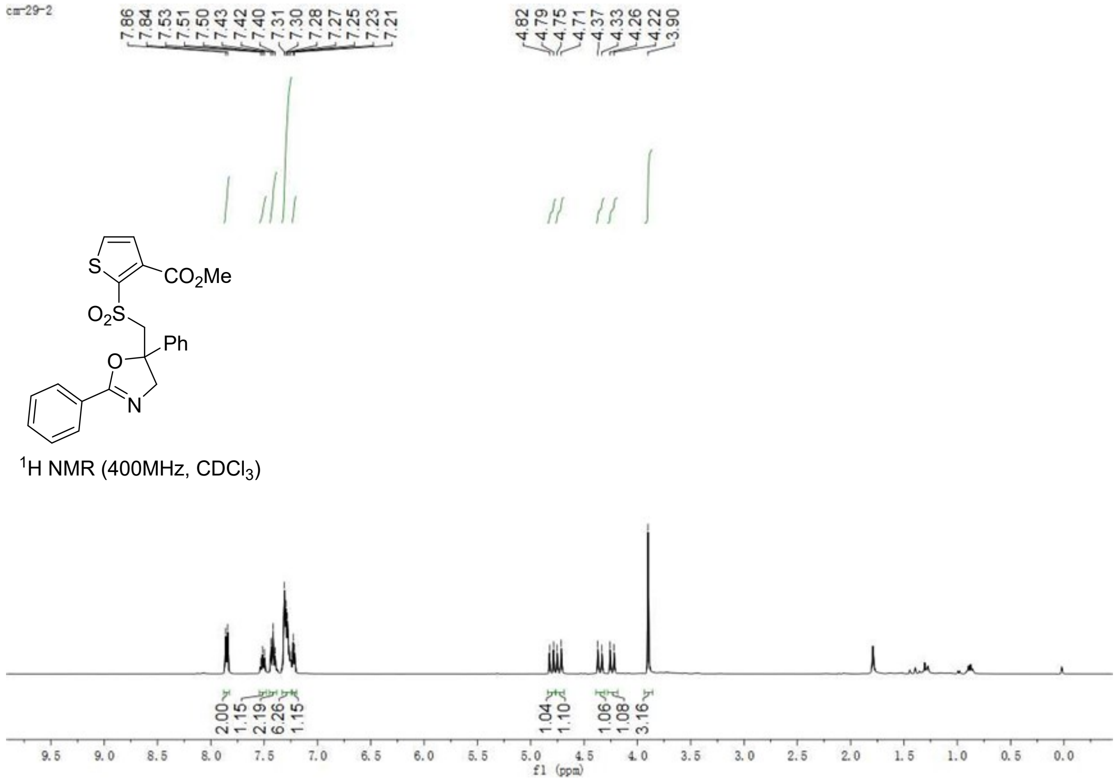
^{1}H NMR spectrum of **3an**



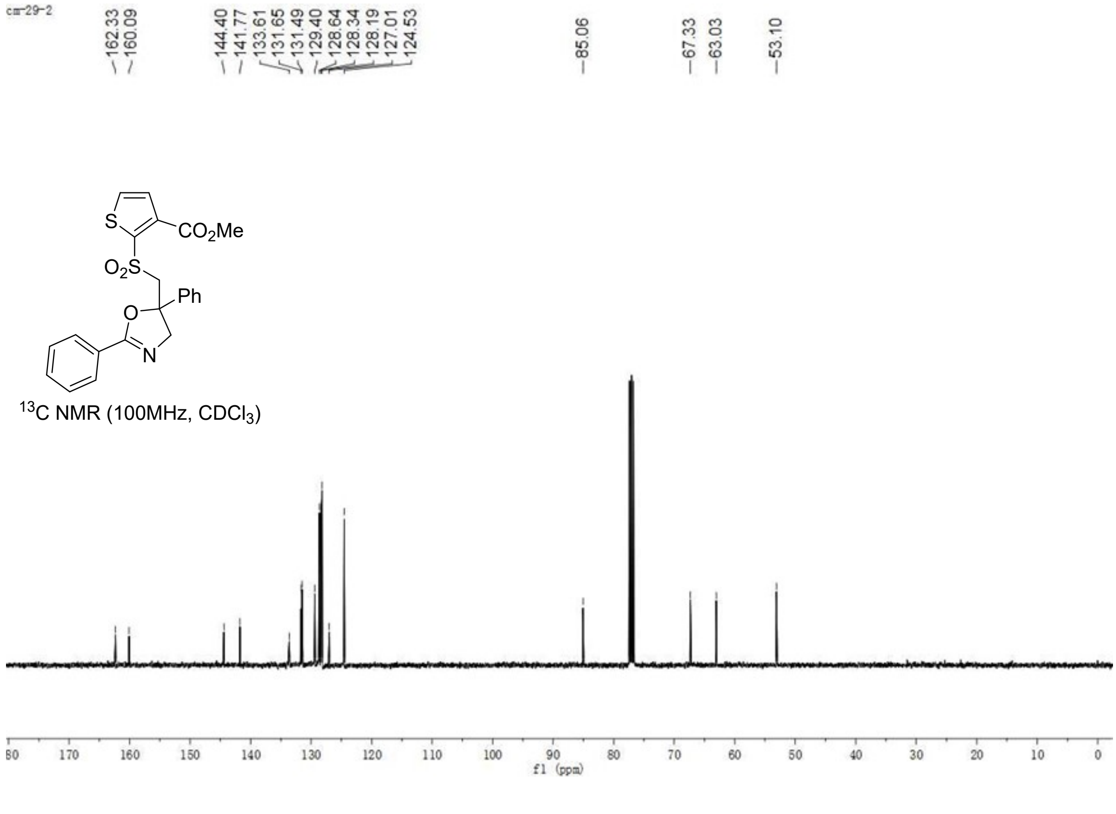
^{13}C NMR spectrum of **3an**



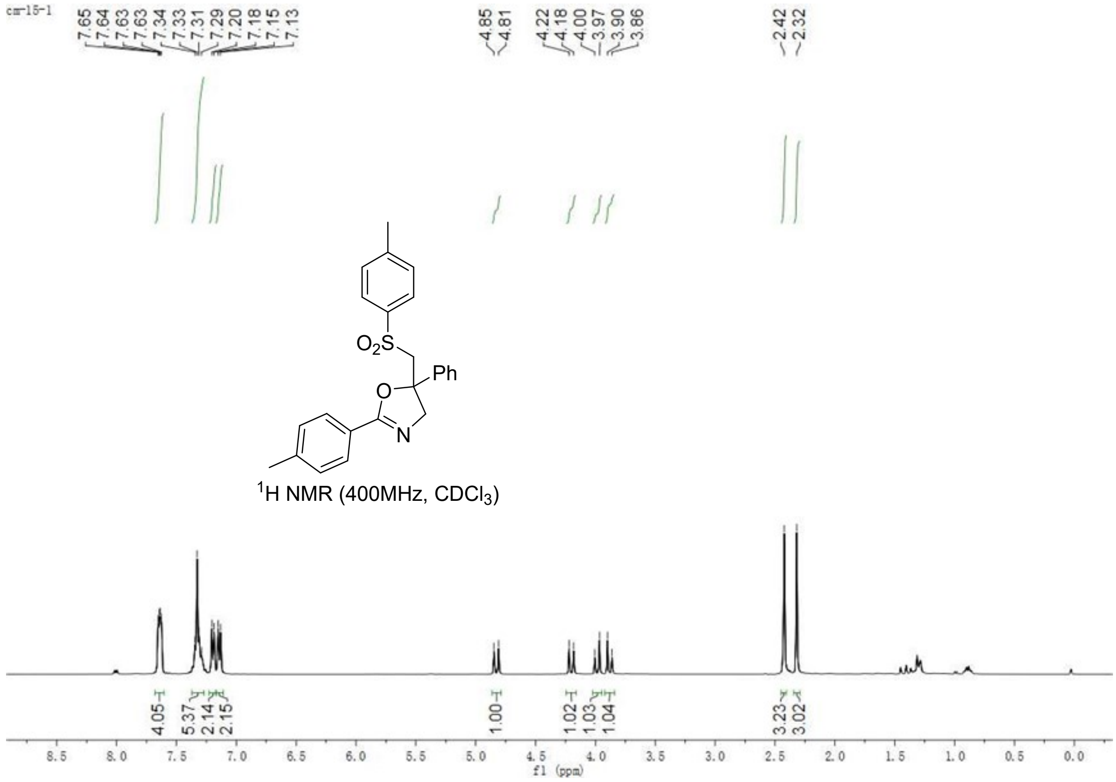
[1]H NMR spectrum of **3ao**



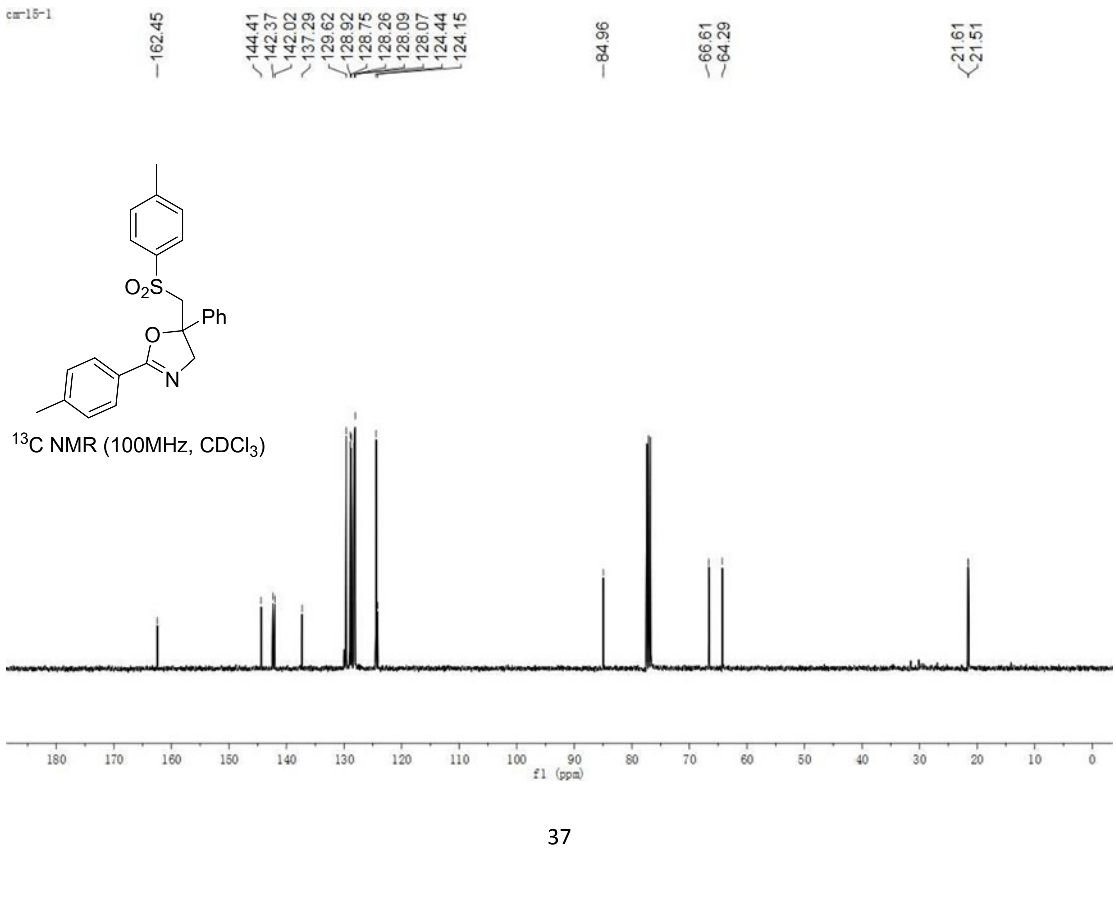
[13]C NMR spectrum of **3ao**



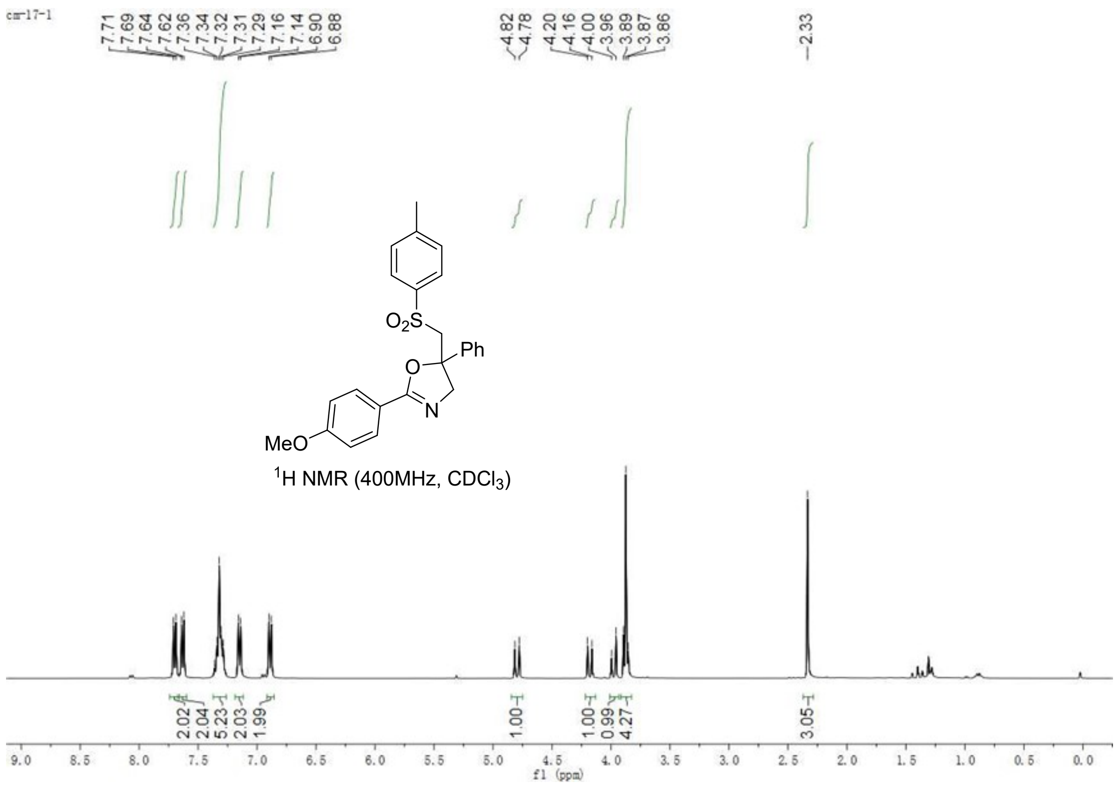
^{1}H NMR spectrum of **3ba**



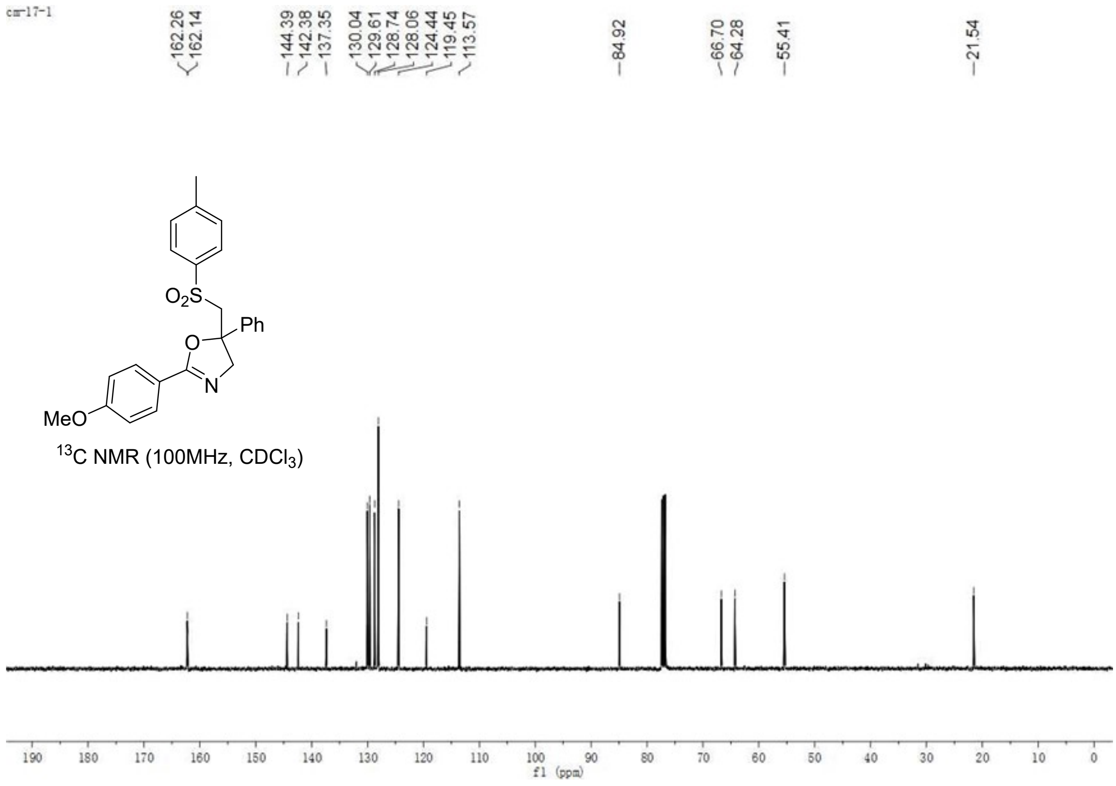
^{13}C NMR spectrum of **3ba**



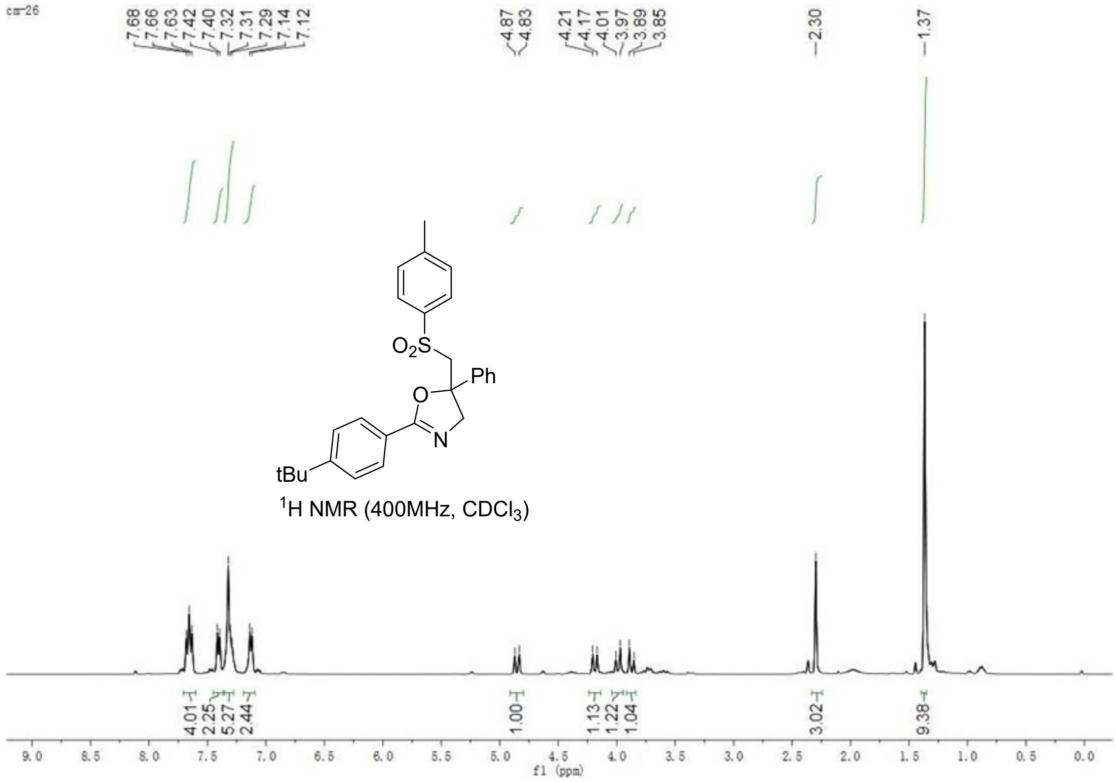
^1H NMR spectrum of **3ca**



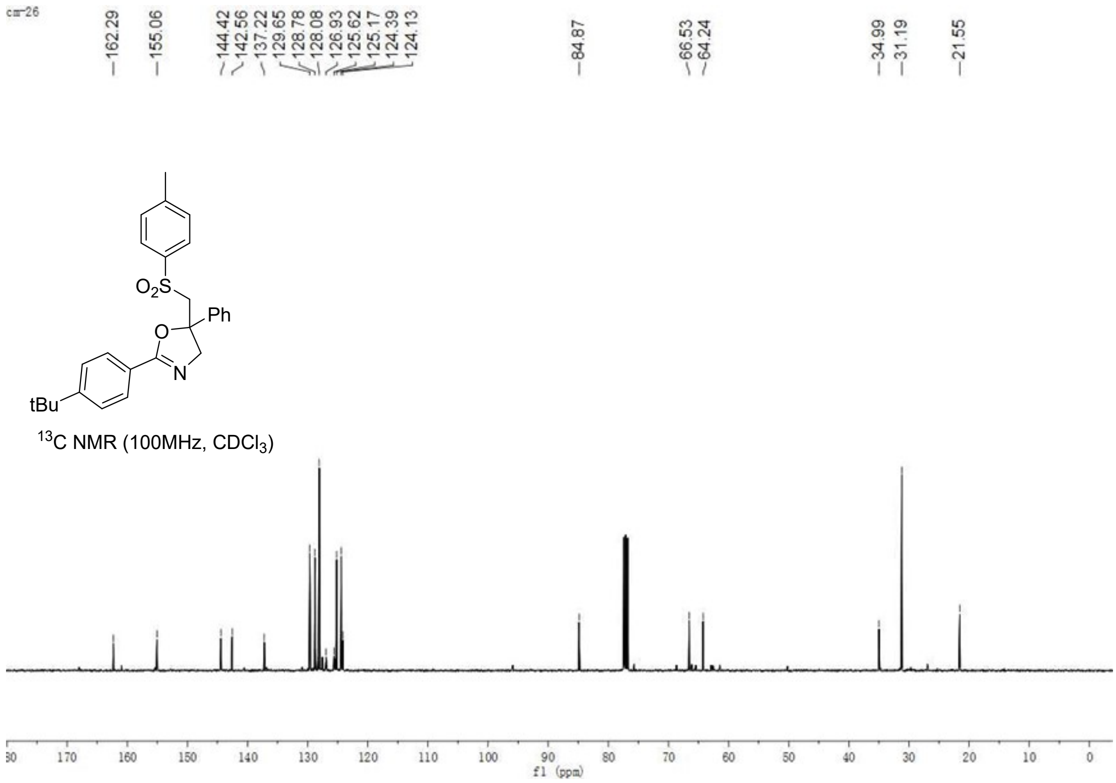
^{13}C NMR spectrum of **3ca**



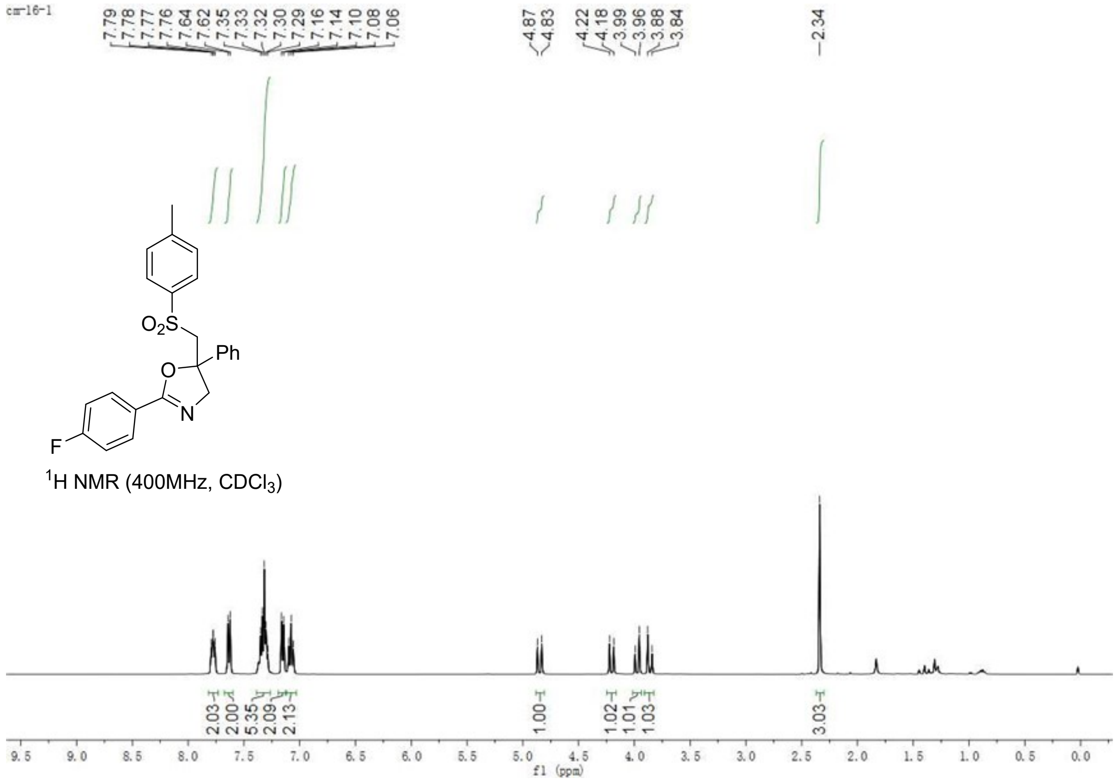
^{1}H NMR spectrum of **3da**



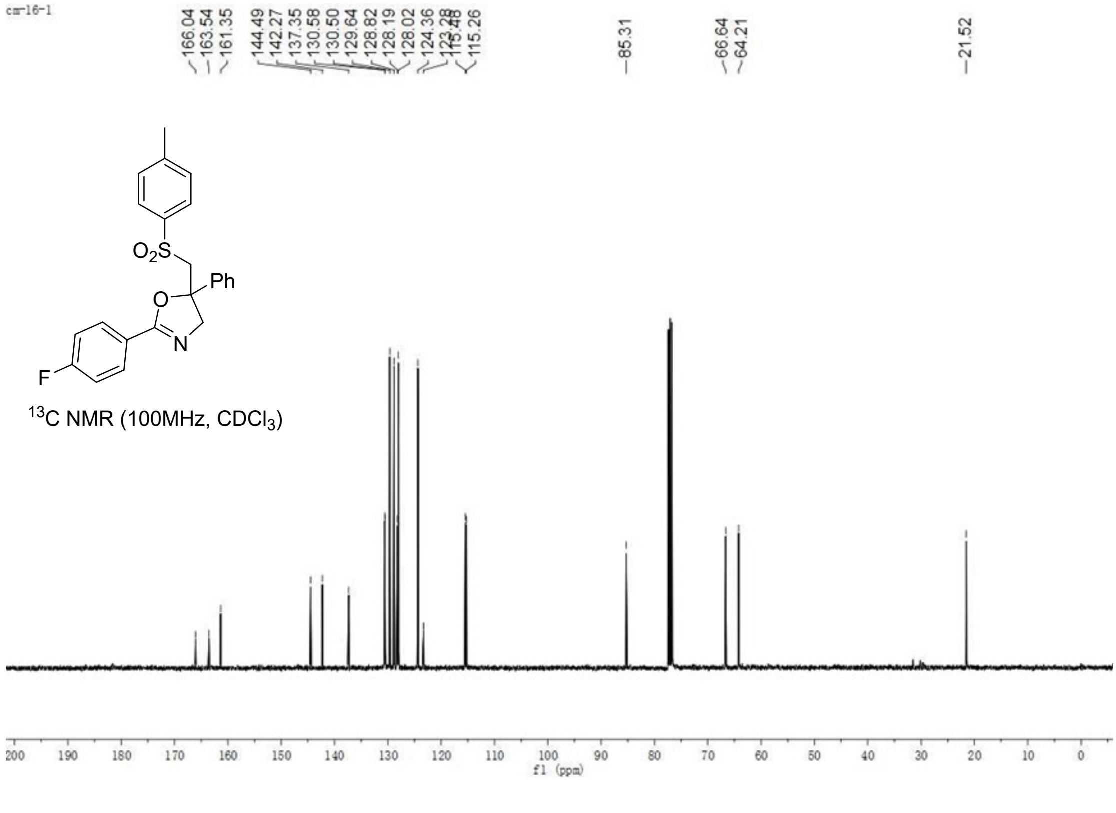
^{13}C NMR spectrum of **3da**



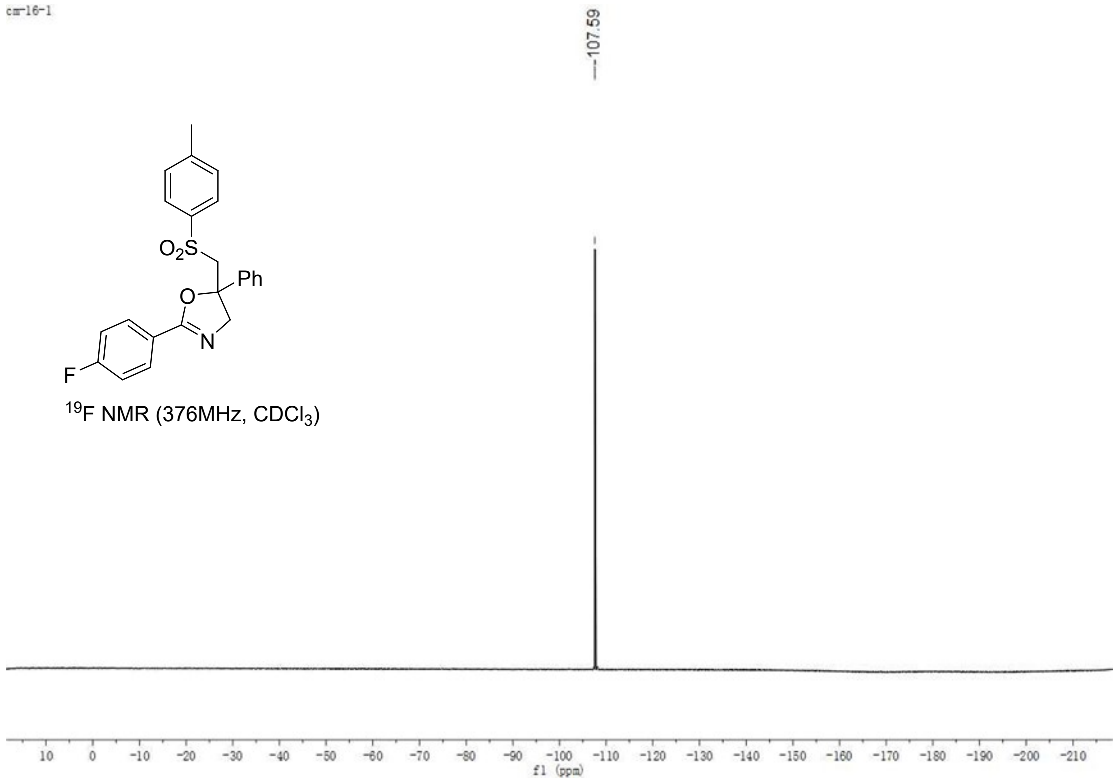
^1H NMR spectrum of **3ea**



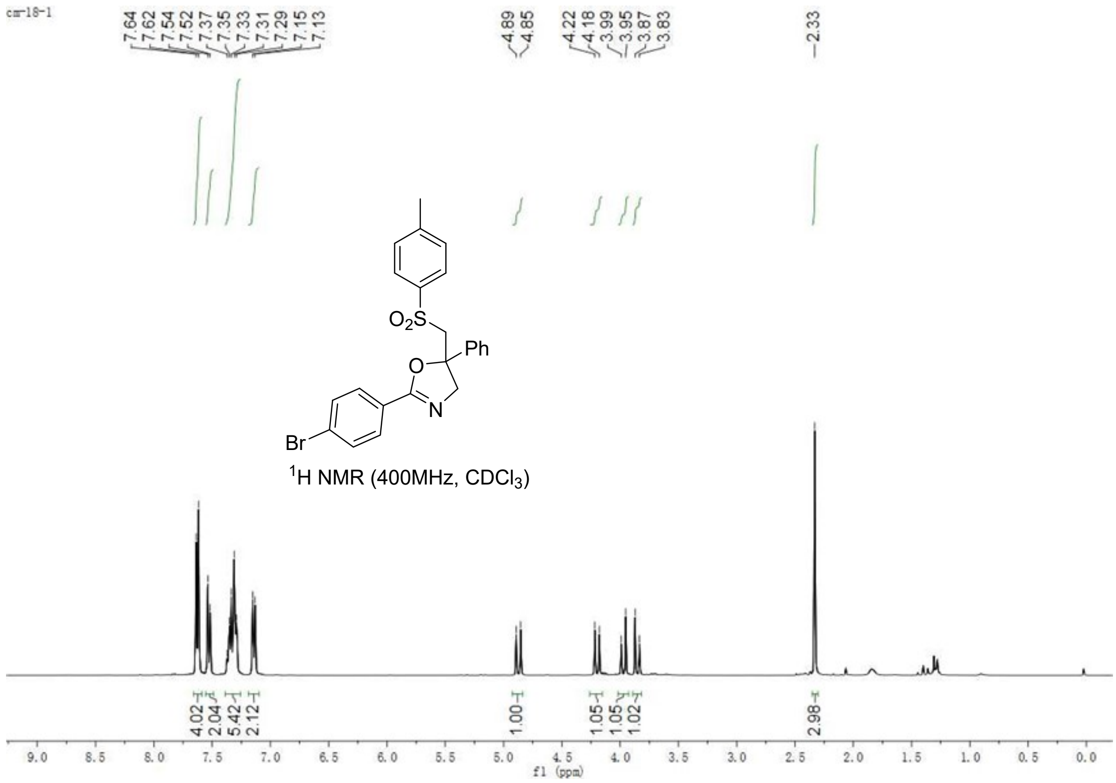
^{13}C NMR spectrum of **3ea**



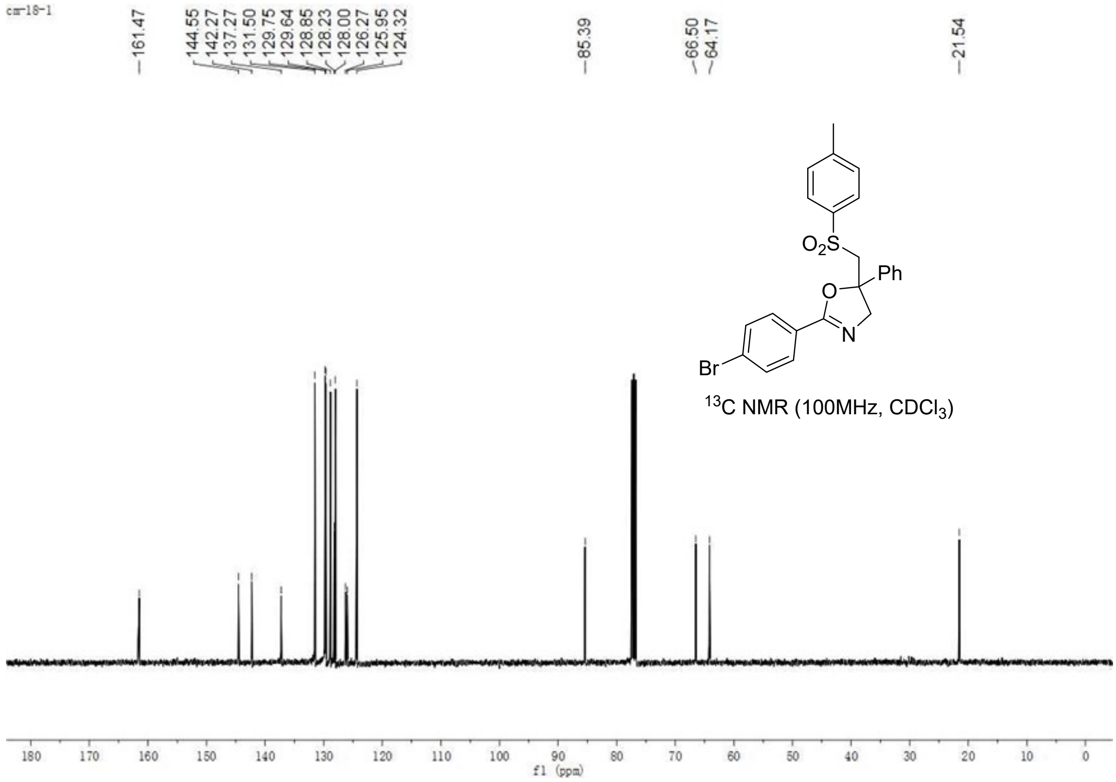
^{19}F NMR spectrum of **3ea**



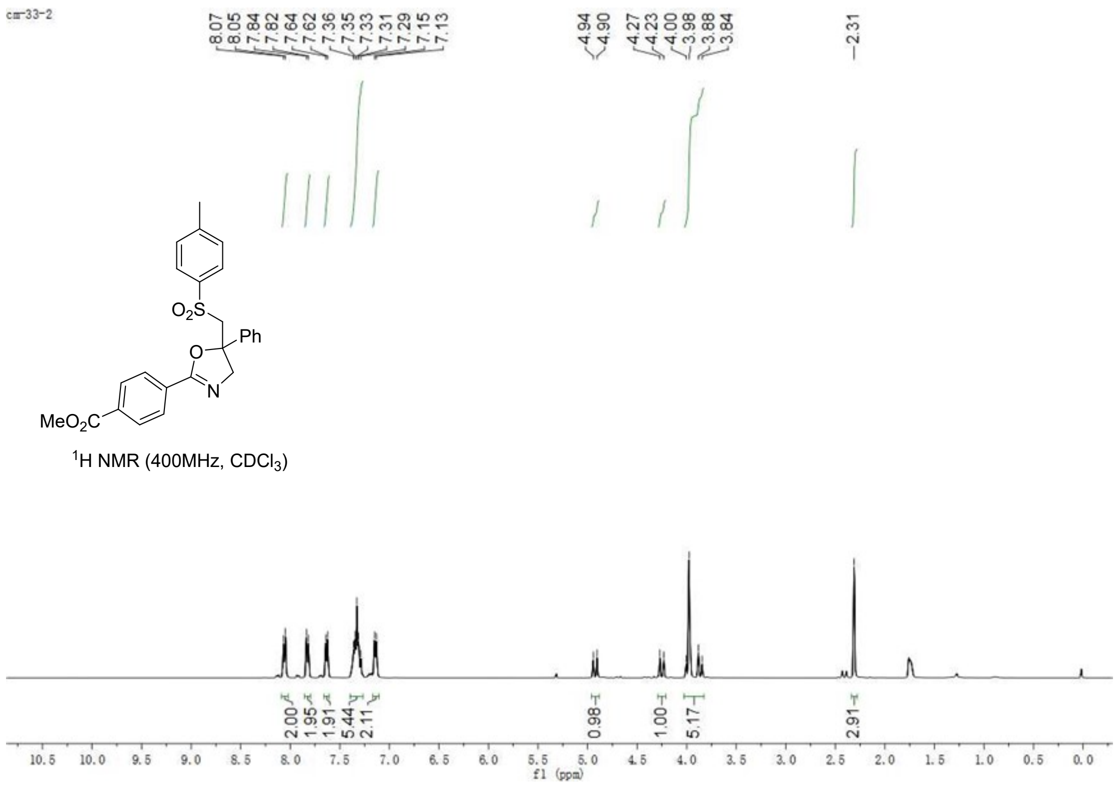
^{1}H NMR spectrum of **3fa**



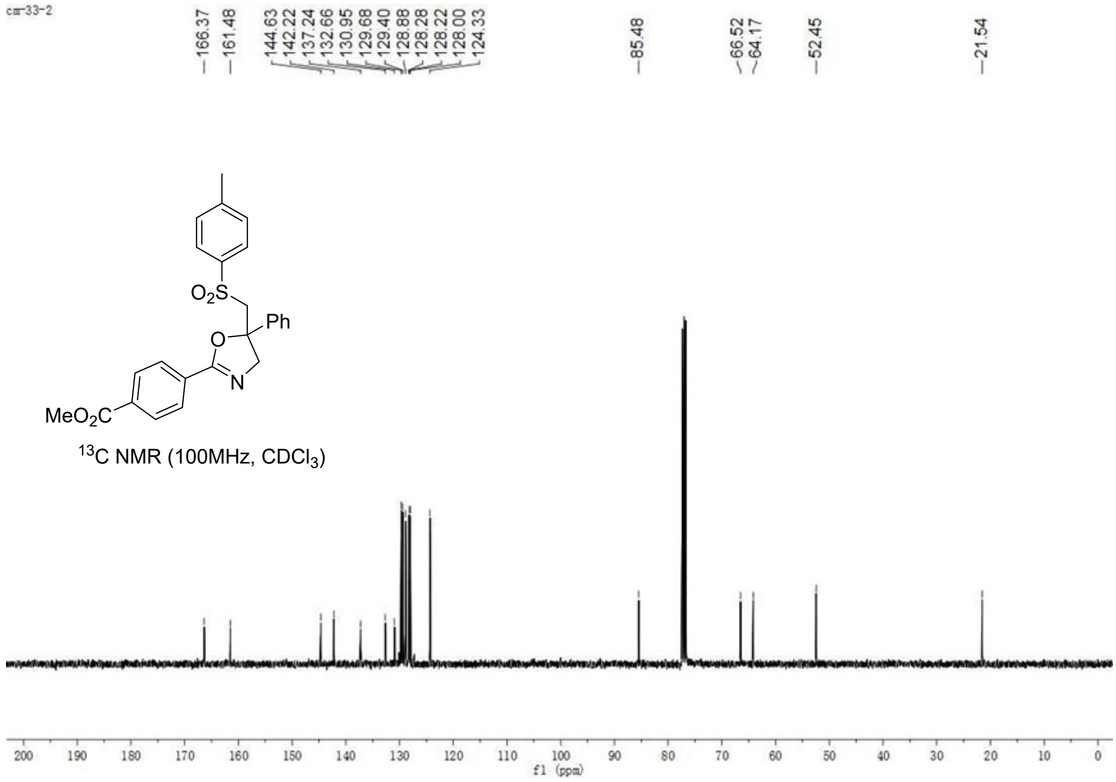
^{13}C NMR spectrum of **3fa**



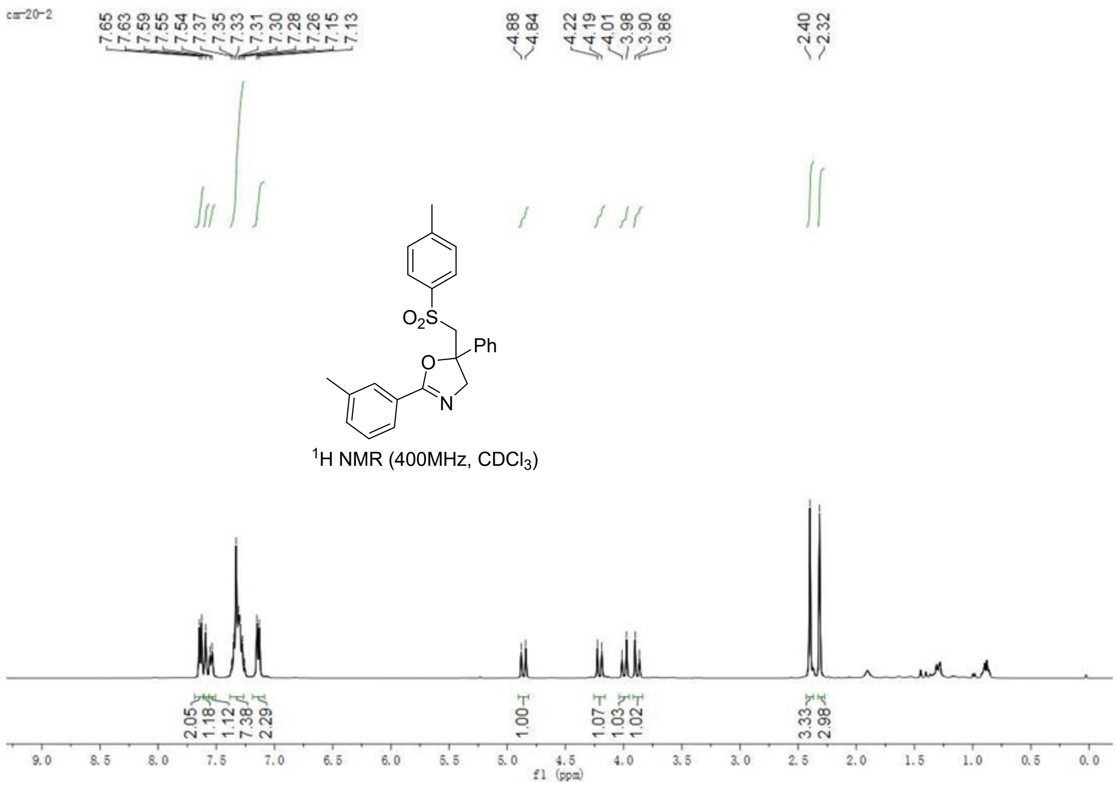
^{1}H NMR spectrum of **3ga**



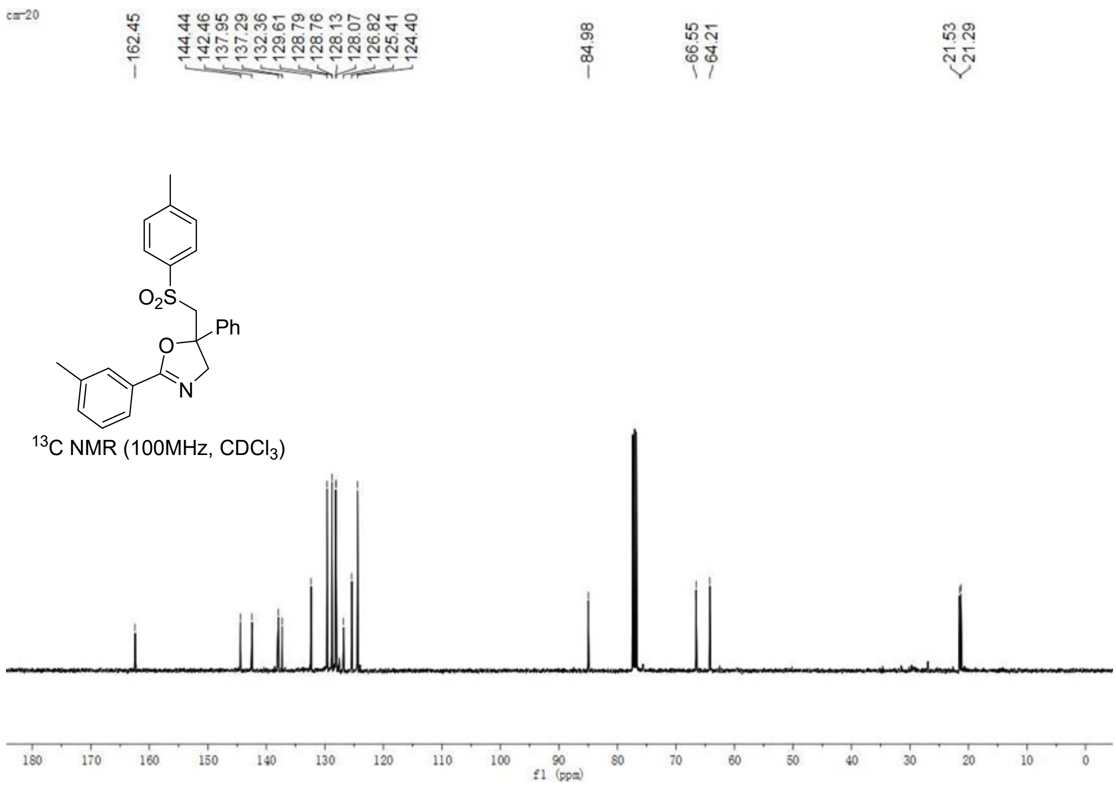
^{13}C NMR spectrum of **3ga**



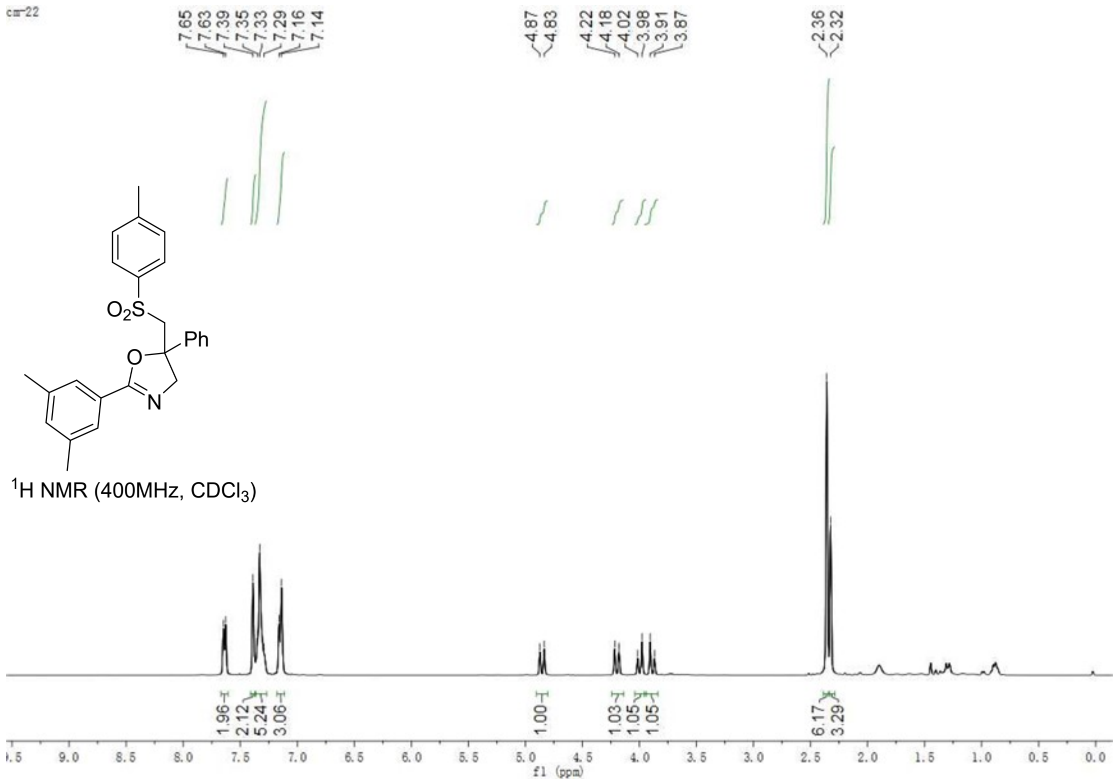
^{1}H NMR spectrum of **3ha**



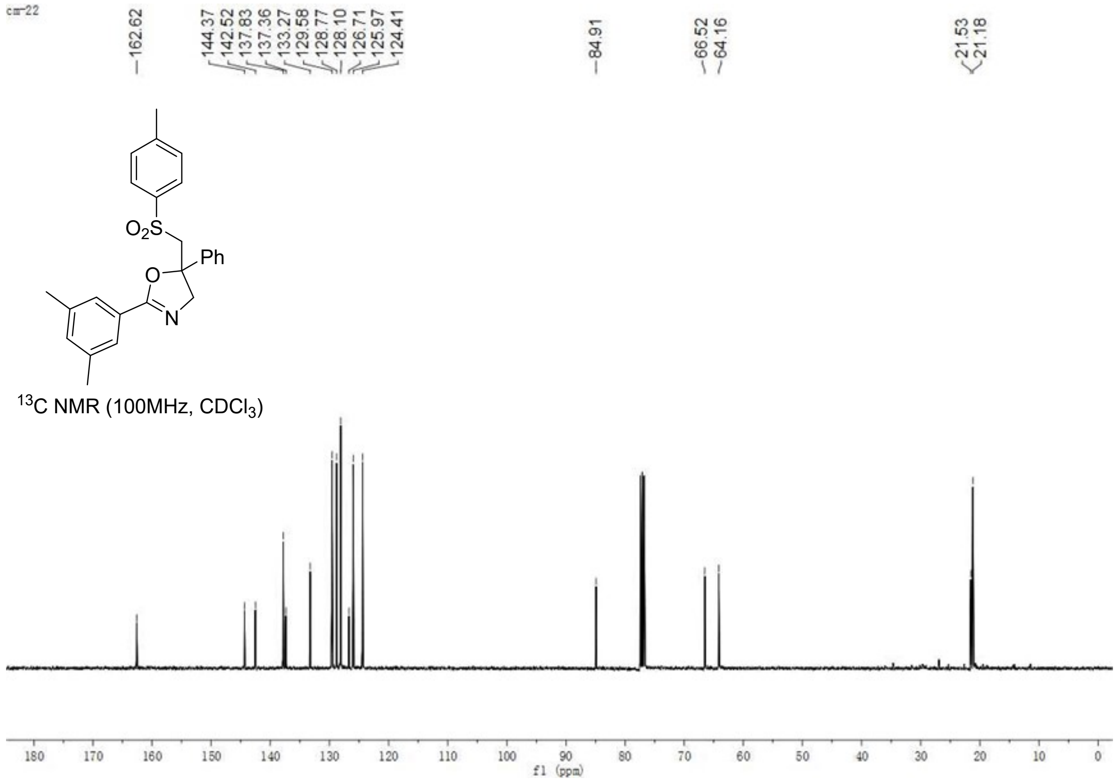
^{13}C NMR spectrum of **3ha**



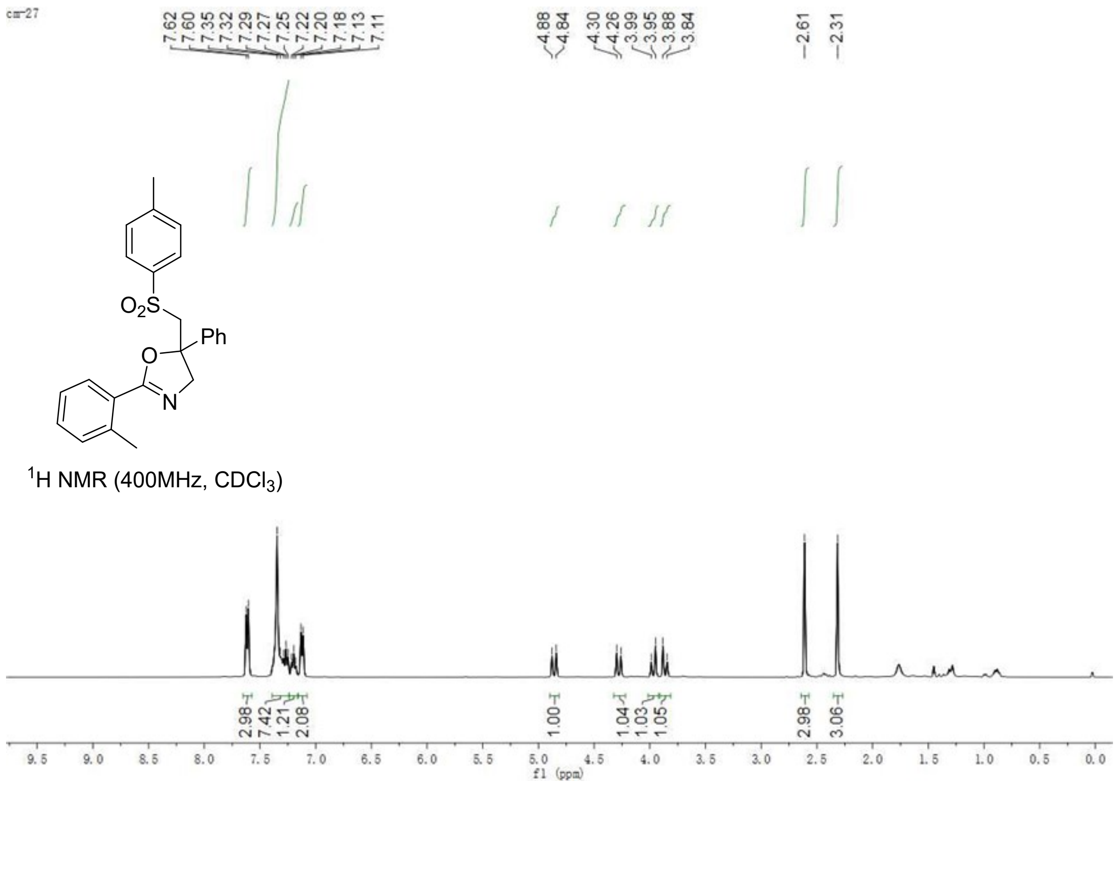
^{1}H NMR spectrum of **3ia**



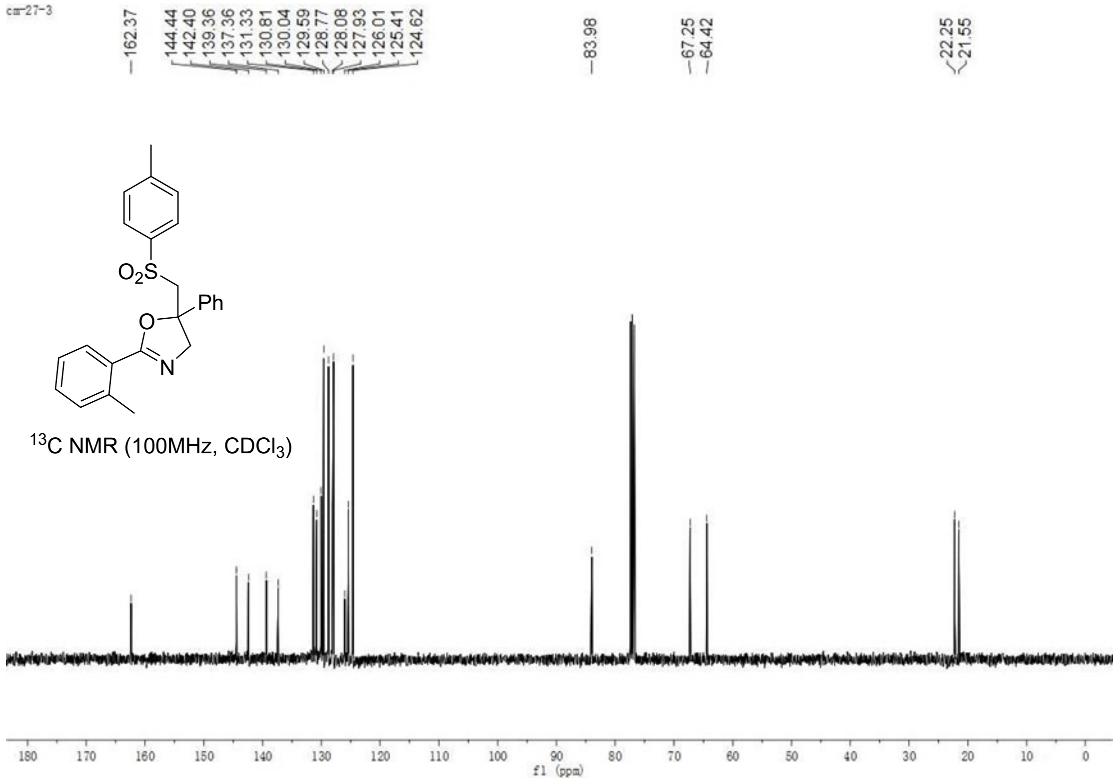
^{13}C NMR spectrum of **3ia**



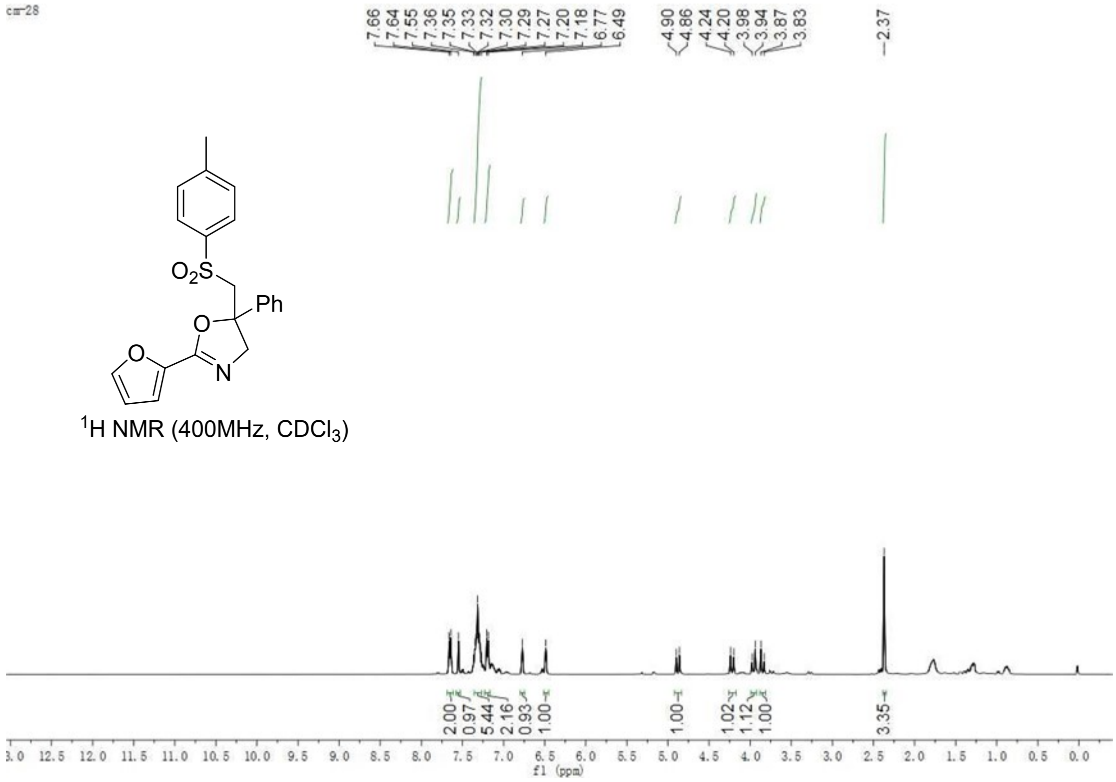
^{1}H NMR spectrum of **3ja**



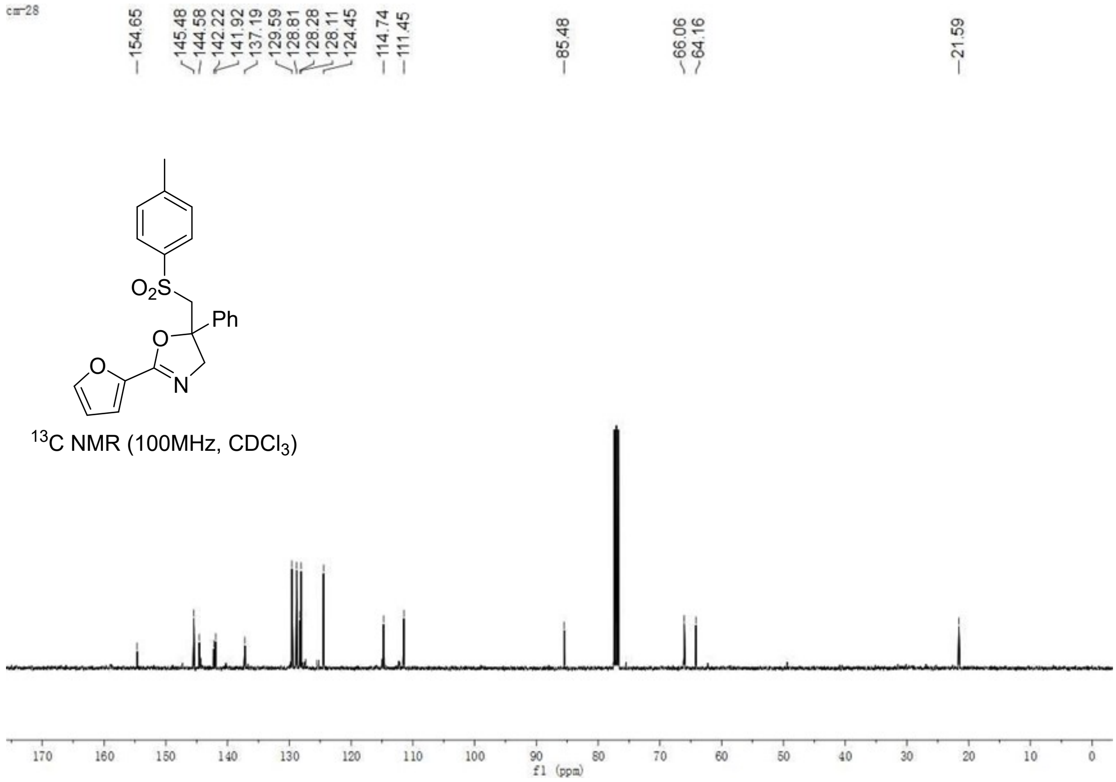
^{13}C NMR spectrum of **3ja**



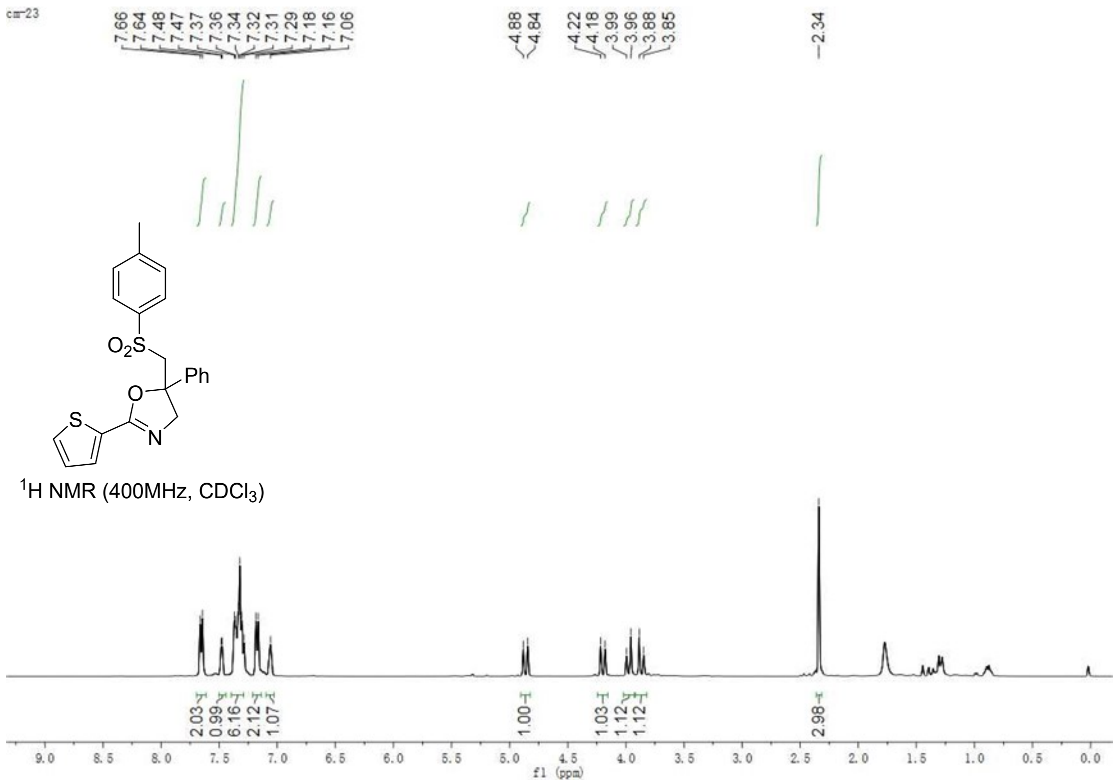
^{1}H NMR spectrum of **3ka**



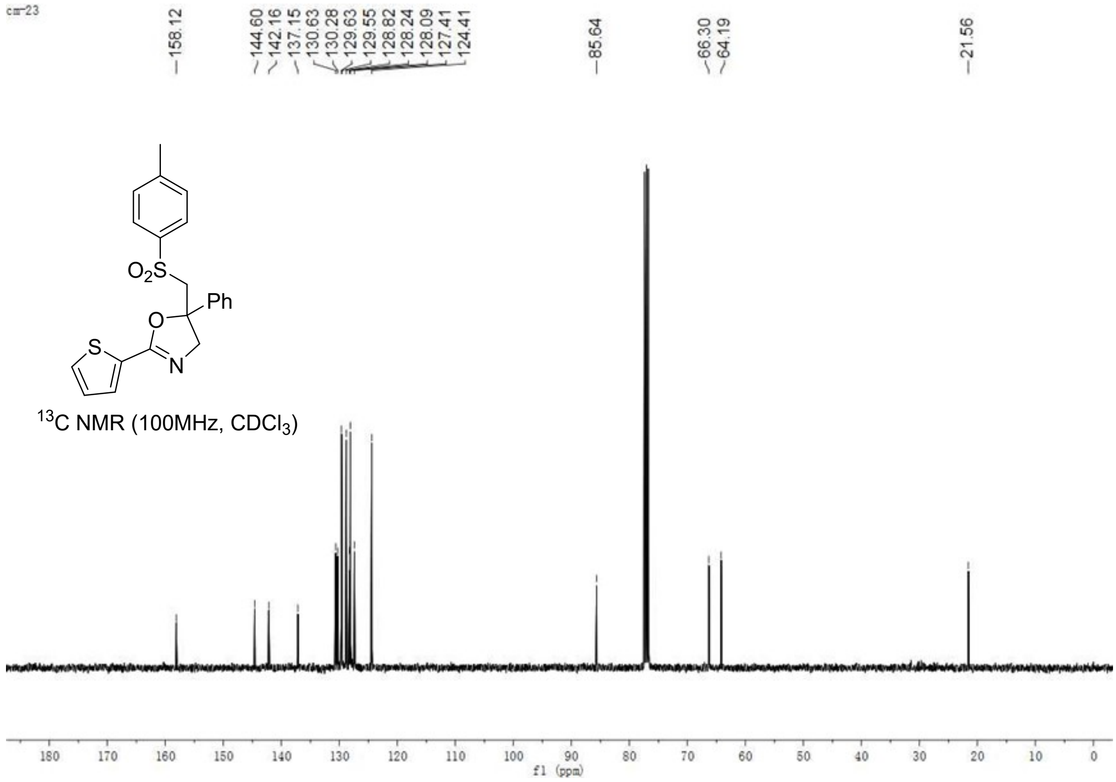
^{13}C NMR spectrum of **3ka**



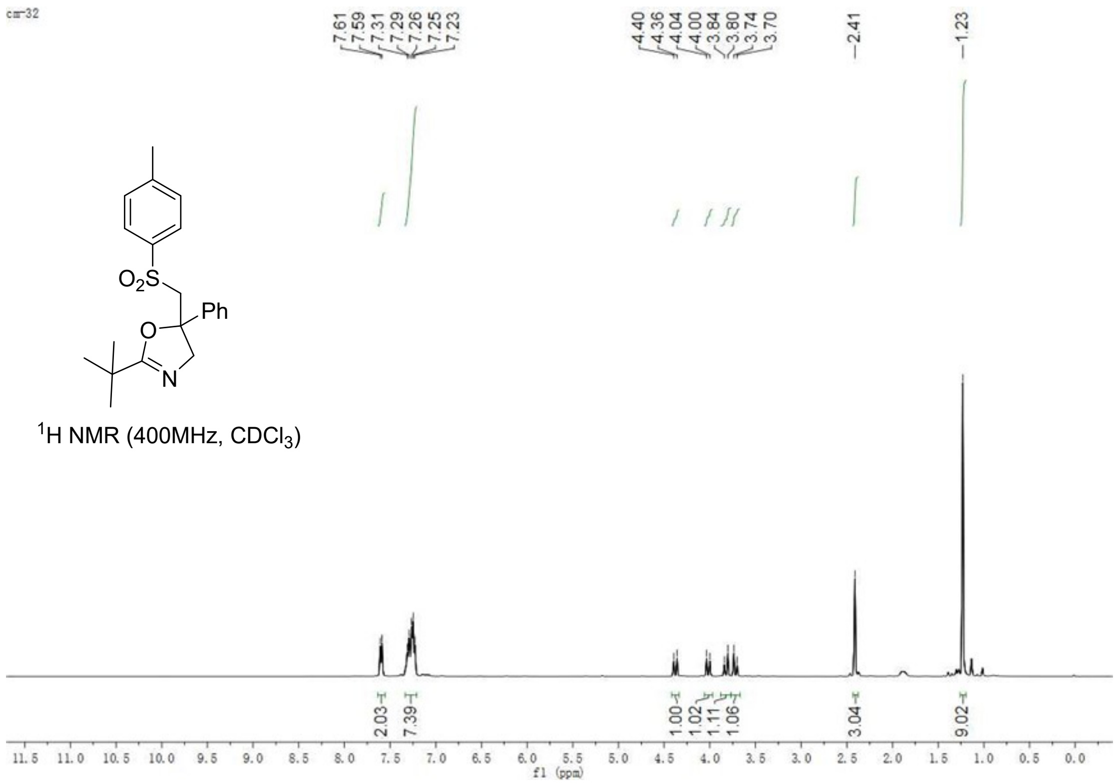
^{1}H NMR spectrum of **3la**



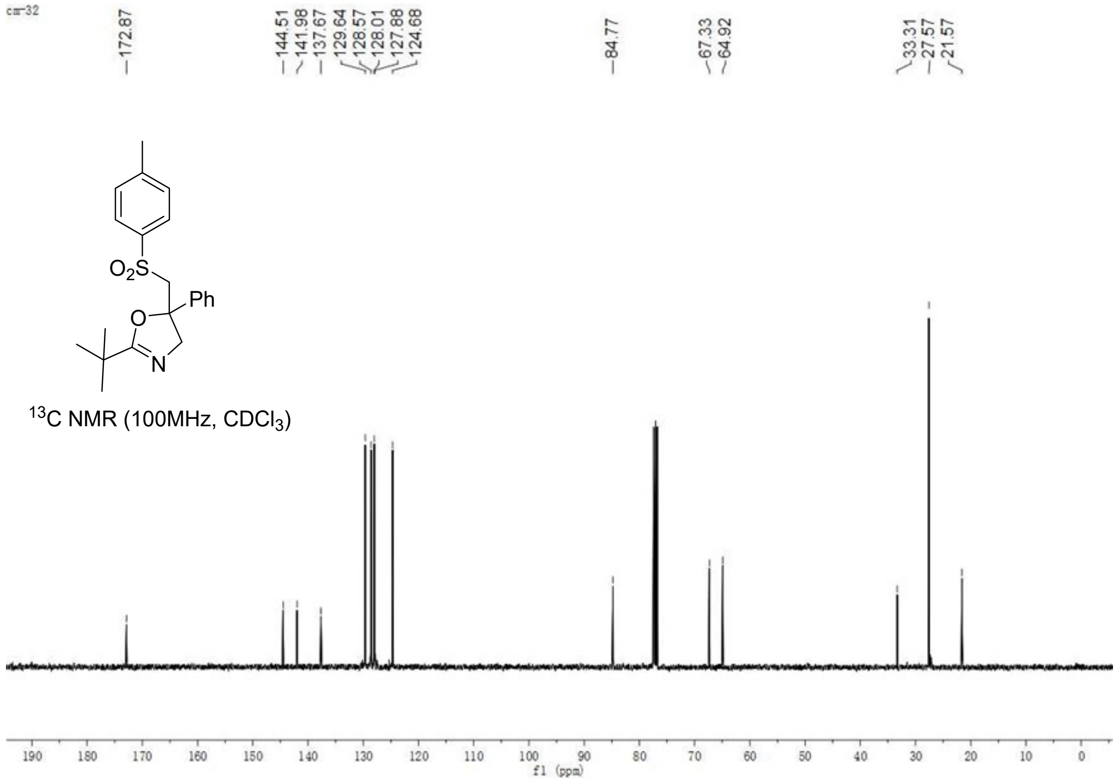
^{13}C NMR spectrum of **3la**



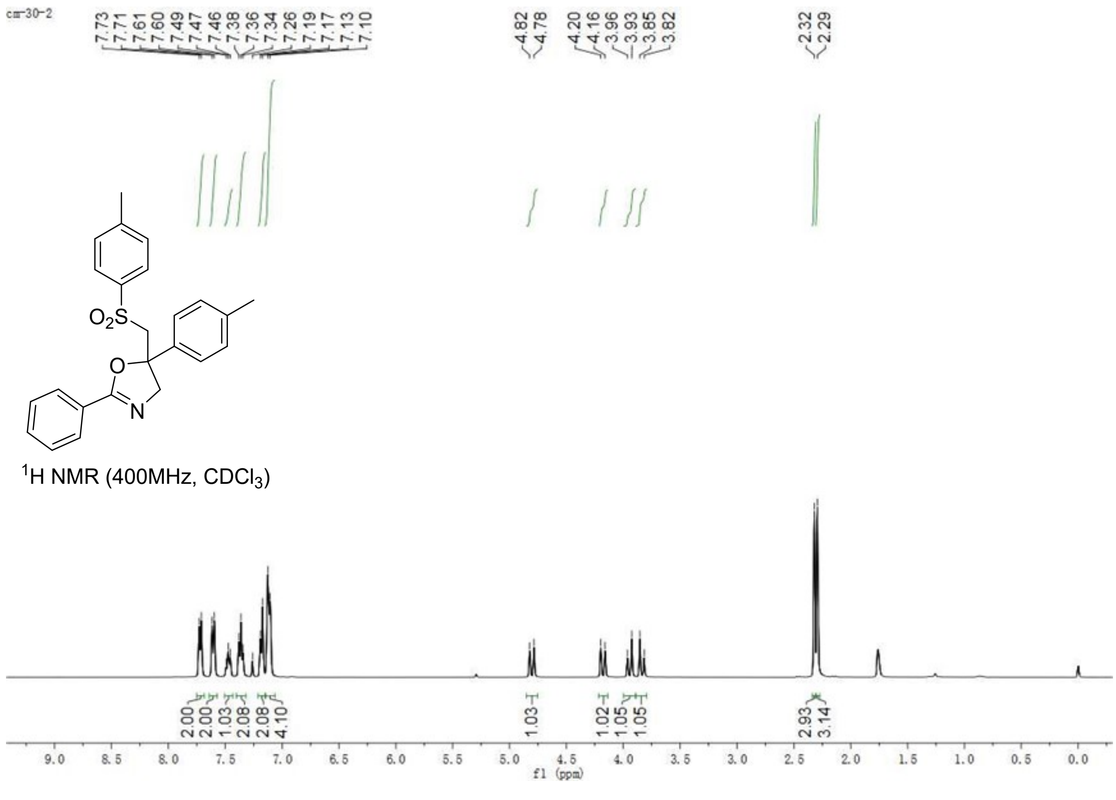
^{1}H NMR spectrum of **3ma**



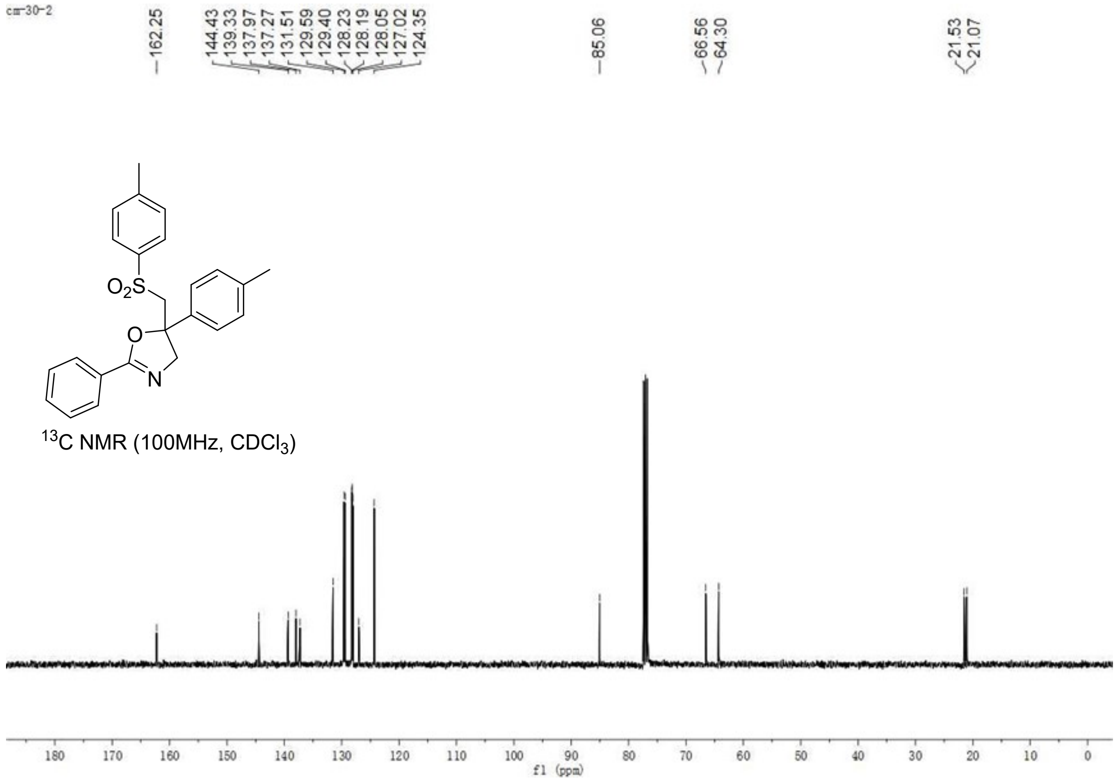
^{13}C NMR spectrum of **3ma**



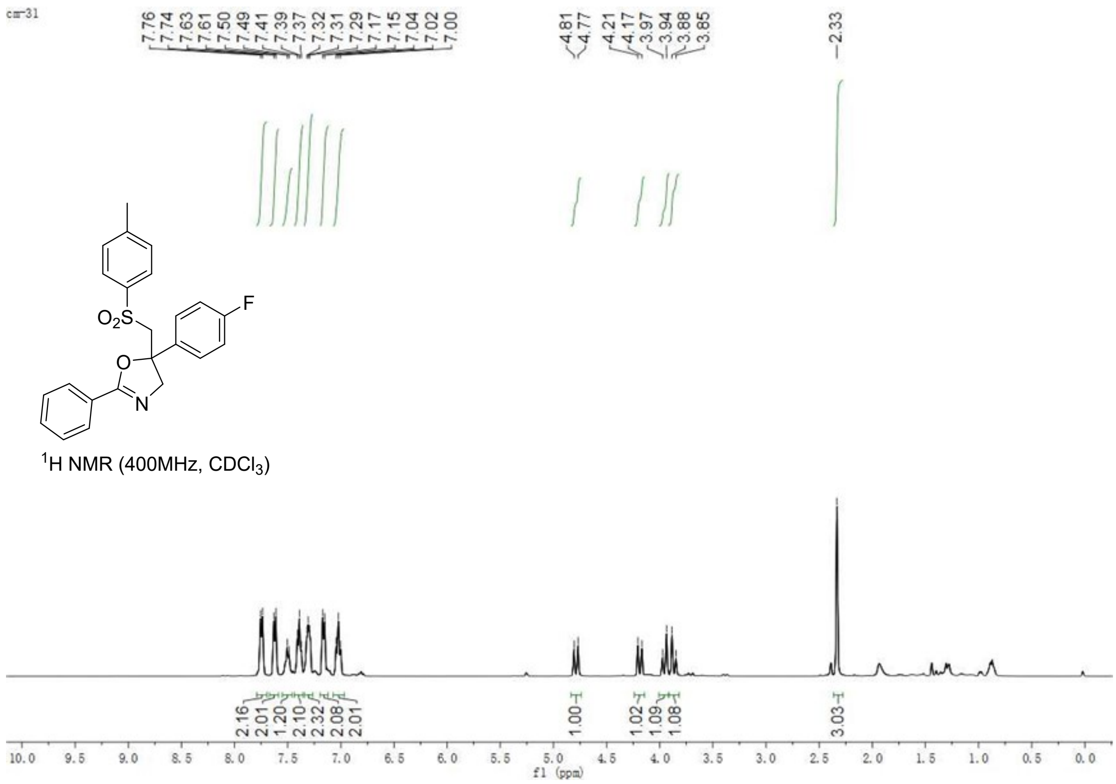
^{1}H NMR spectrum of **3na**



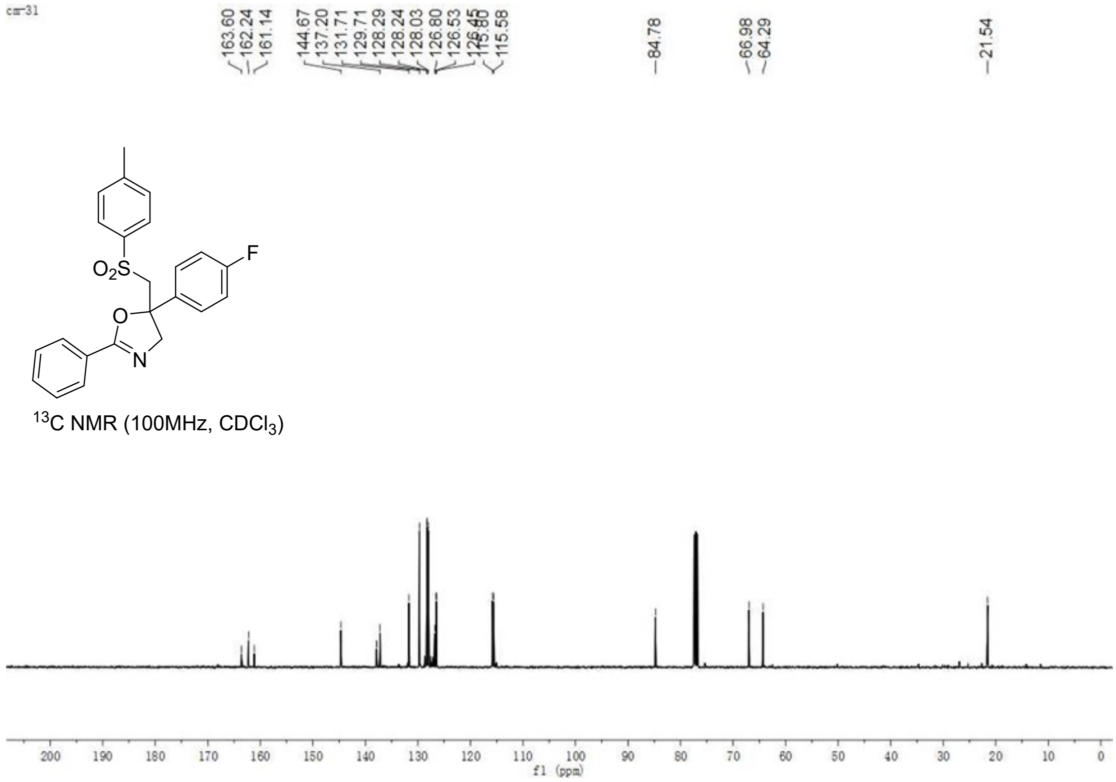
^{13}C NMR spectrum of **3na**



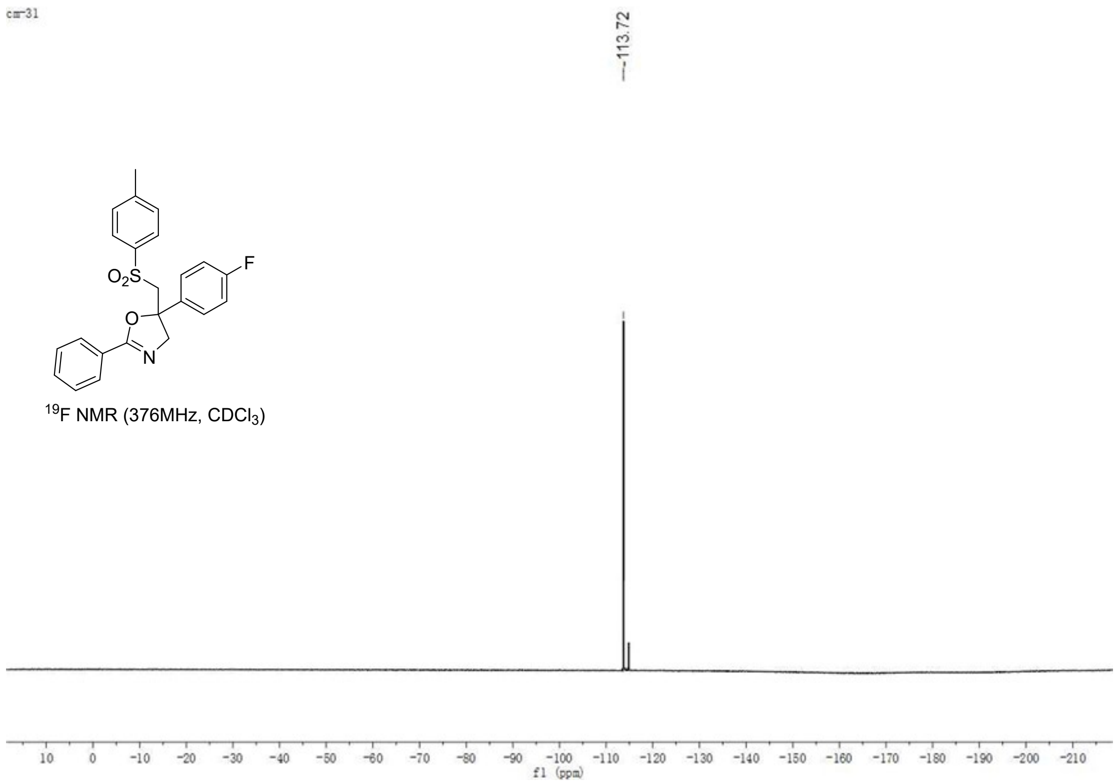
^{1}H NMR spectrum of **3oa**



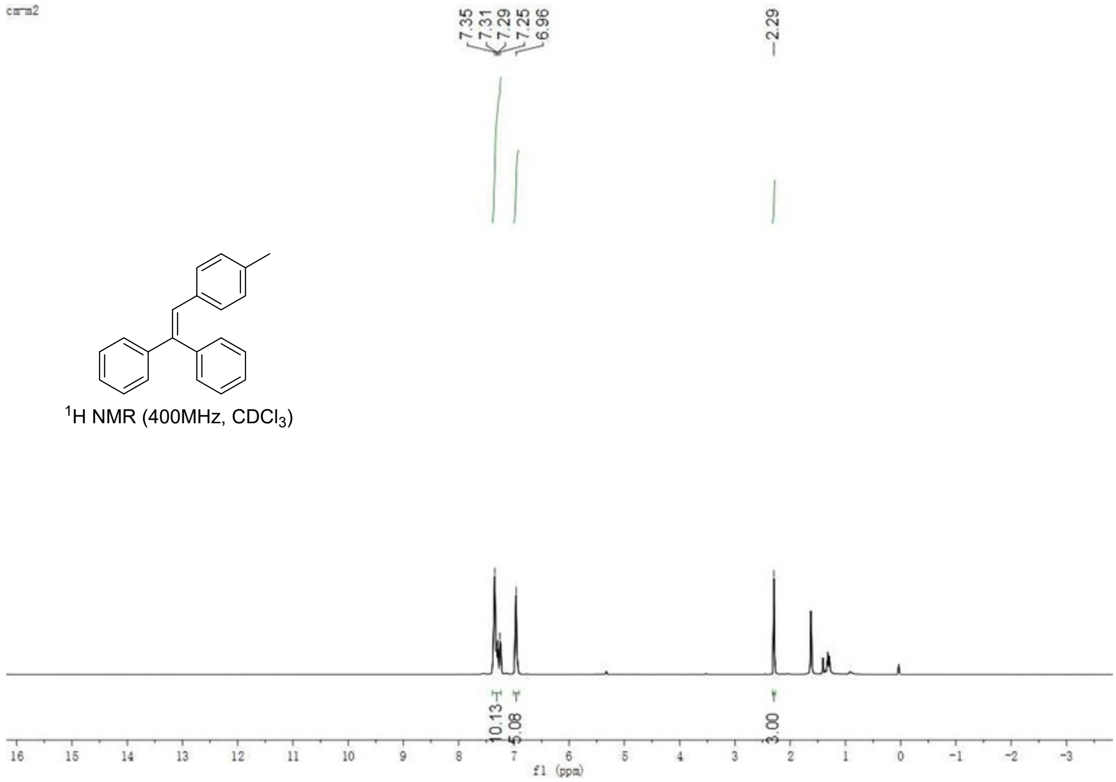
^{13}C NMR spectrum of **3oa**



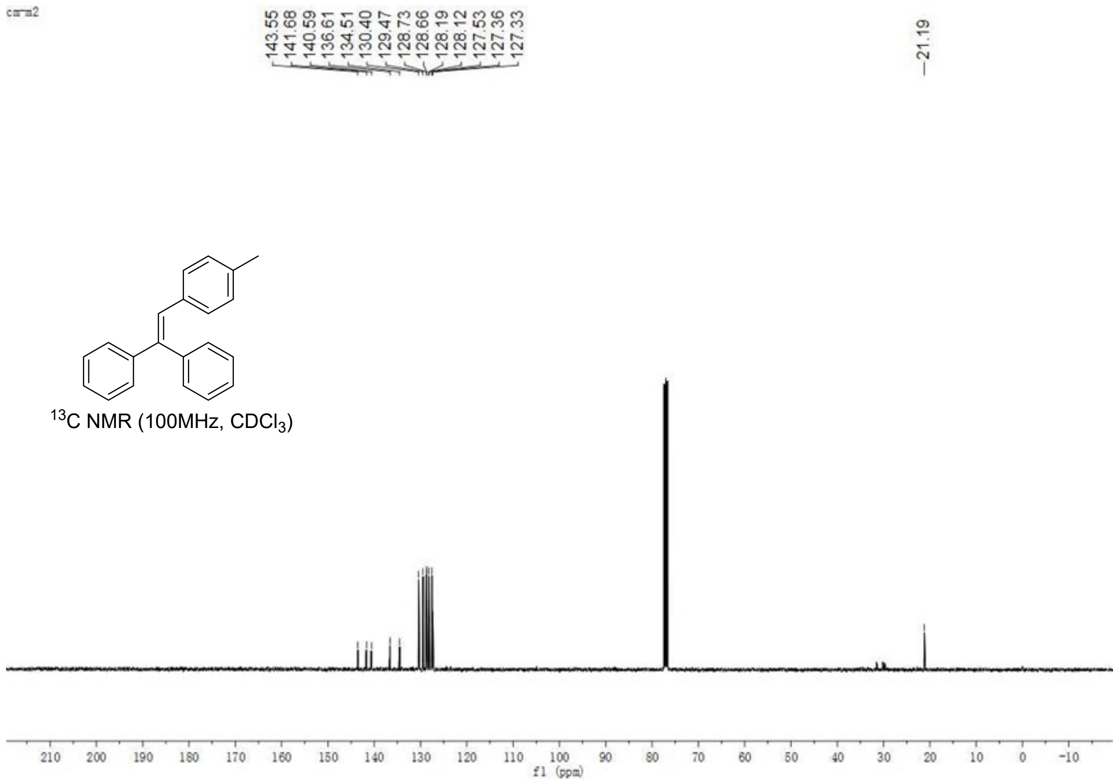
^{19}F NMR spectrum of **3oa**



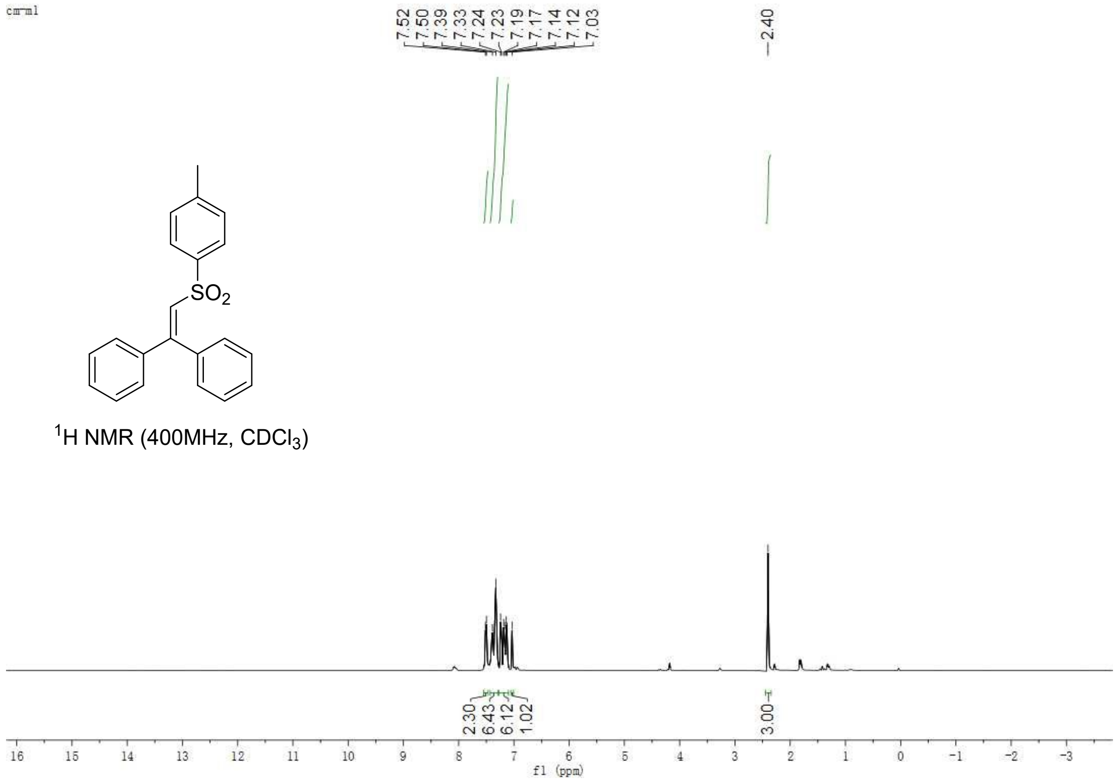
^{1}H NMR spectrum of **4**



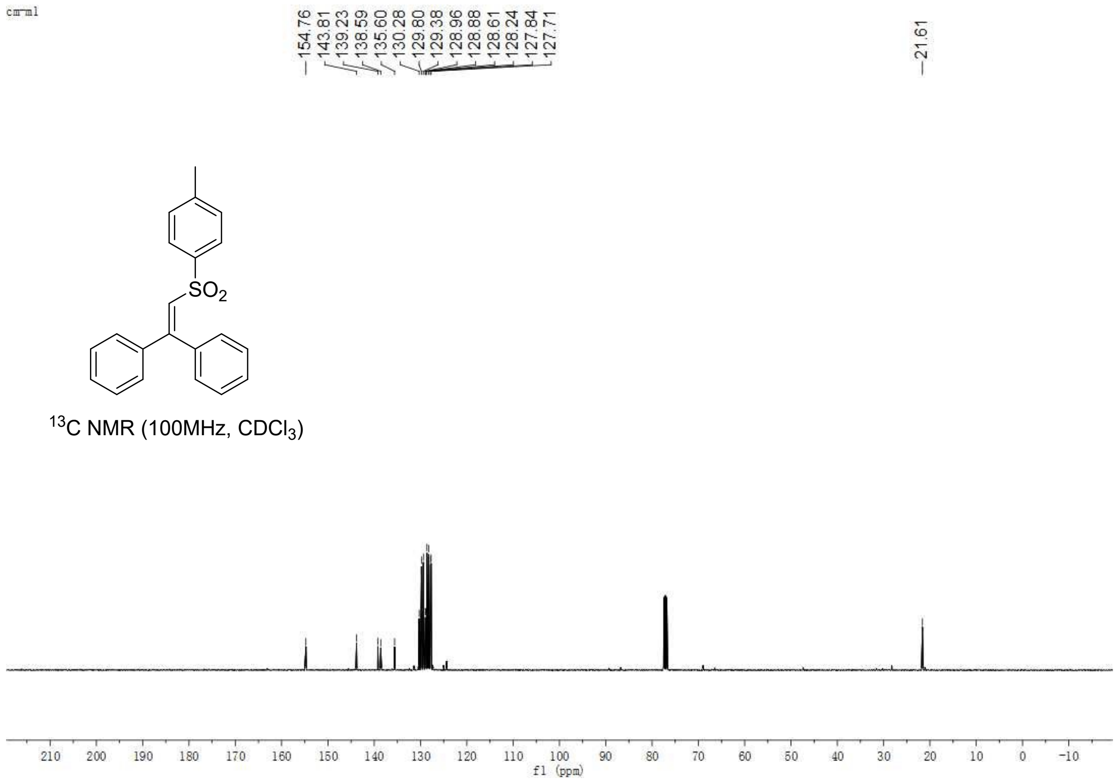
^{13}C NMR spectrum of **4**



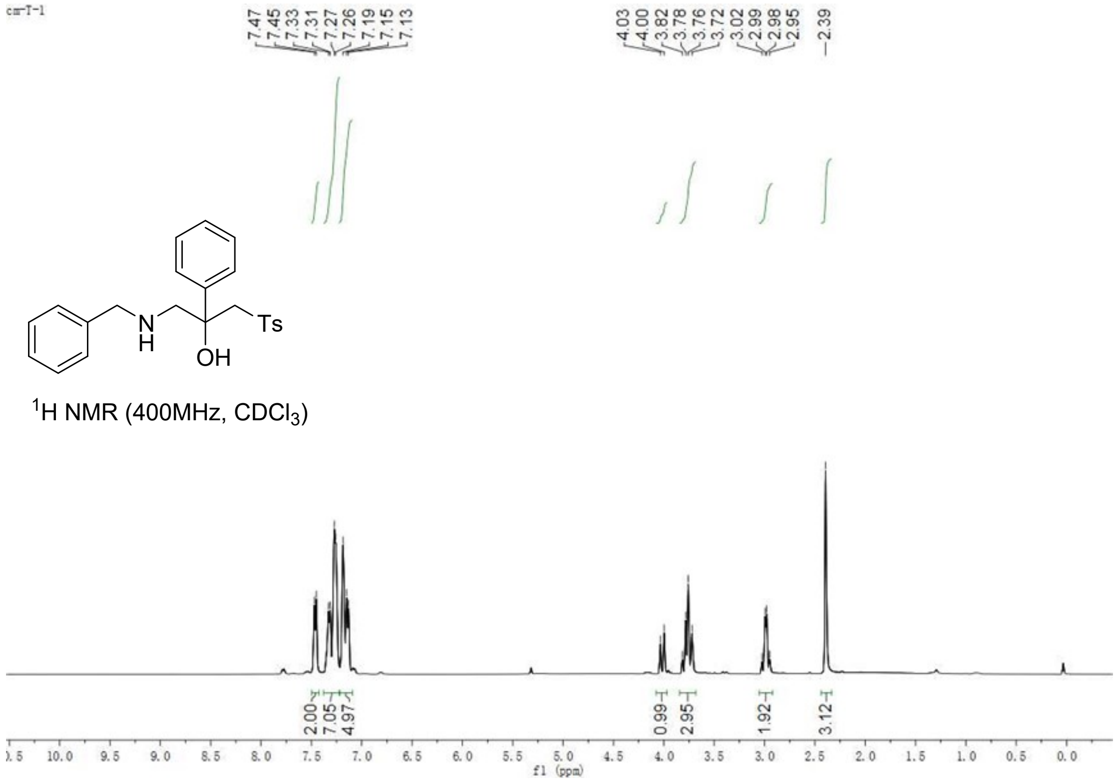
^{1}H NMR spectrum of **5**



^{13}C NMR spectrum of **5**



^{1}H NMR spectrum of **6**



^{13}C NMR spectrum of **6**